

10/596571

=> file registry

FILE 'REGISTRY' ENTERED AT 13:20:06 ON 04 JAN 2010

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0

DICTIONARY FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

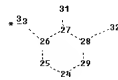
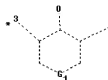
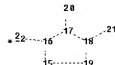
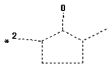
Uploading L3.str



G₂



56



10/596571

```
11 12 13 14 20 21 22 23 31 32 49 50 51 52 56
ring nodes :
1 2 3 4 5 6 15 16 17 18 19 24 25 26 27 28 29 35 36 37 38 39
40 41 42 43 44 45 46 47 48
ring/chain nodes :
7 8 9
chain bonds :
11-12 11-13 13-14 16-22 17-20 18-21 23-26 27-31 28-32 37-51 38-49 45-50
46-52
ring/chain bonds :
7-8 7-9
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-19 16-17 17-18 18-19 24-25 24-29 25-
26
26-27 27-28 28-29 35-36 35-40 36-37 37-38 38-39 39-40 39-41 40-44 41-42
42-43 42-45
43-44 43-48 45-46 46-47 47-48
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 11-12 11-13 13-14 15-16 15-19 16-17
16-22 17-18 17-20 18-19 18-21 23-26 24-25 24-29 25-26 26-27 27-28 27-31
28-29 28-32
35-36 35-40 36-37 37-38 37-51 38-39 38-49 39-40 39-41 40-44 41-42 42-43
42-45 43-44 43-48
45-46 45-50 46-47 46-52 47-48
```

G1:C,N

G2:[*1],[*2],[*3],[*4]

```
Connectivity :
15:2 E exact RC ring/chain 16:3 E exact RC ring/chain 17:3 E exact RC ring/chain
18:3 E exact RC ring/chain 19:2 E exact RC ring/chain 20:1 E exact RC ring/chain
21:2 X maximum
RC ring/chain 22:2 E exact RC ring/chain 23:2 E exact RC ring/chain 25:2 E exact
RC ring/chain
26:3 E exact RC ring/chain 27:3 E exact RC ring/chain 28:3 E exact RC ring/chain
29:2 E exact
RC ring/chain 31:1 E exact RC ring/chain 32:2 X maximum RC ring/chain 38:3 E
exact RC ring/chain
45:3 E exact RC ring/chain 46:3 E exact RC ring/chain 49:1 E exact RC ring/chain
50:1 E exact
RC ring/chain 51:2 E exact RC ring/chain 52:2 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS
22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:CLASS
32:CLASS 35:Atom
36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom
47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 56:CLASS
```

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 13:20:08 ON 04 JAN 2010

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

10/596571

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 4 Jan 2010 VOL 152 ISS 2
FILE LAST UPDATED: 3 Jan 2010 (20100103/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

ZCaplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

```
=> d stat que L35
L3          STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
```

Structure attributes must be viewed using STN Express query preparation.

```
L7          995 SEA FILE=REGISTRY SSS FUL L3
L34         4245 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  KHAN S?/AU,AUTH
L35         5 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L7 AND L34
```

```
=> d stat que L37
L34         4245 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  KHAN S?/AU,AUTH
L36         10335 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  BORONIC ACID?/BI
L37         4 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L34 AND L36
```

```
=> s L35 or L37
L39         6 L35 OR L37
```

```
=> file medline embase biosis wpix
FILE 'MEDLINE' ENTERED AT 13:20:25 ON 04 JAN 2010
```

```
FILE 'EMBASE' ENTERED AT 13:20:25 ON 04 JAN 2010
Copyright (c) 2010 Elsevier B.V. All rights reserved.
```

```
FILE 'BIOSIS' ENTERED AT 13:20:25 ON 04 JAN 2010
Copyright (c) 2010 The Thomson Corporation
```

```
FILE 'WPIX' ENTERED AT 13:20:25 ON 04 JAN 2010
COPYRIGHT (C) 2010 THOMSON REUTERS
```

10/596571

```
=> d stat que L38
L34      4245 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON KHAN S?/AU,AUTH
L38      10 SEA L34 AND BORONIC ACID?
```

```
=> dup rem L39 L38
FILE 'ZCAPLUS' ENTERED AT 13:20:37 ON 04 JAN 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)
```

```
FILE 'MEDLINE' ENTERED AT 13:20:37 ON 04 JAN 2010
```

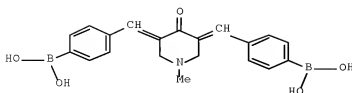
```
FILE 'EMBASE' ENTERED AT 13:20:37 ON 04 JAN 2010
Copyright (c) 2010 Elsevier B.V. All rights reserved.
```

```
FILE 'BIOSIS' ENTERED AT 13:20:37 ON 04 JAN 2010
Copyright (c) 2010 The Thomson Corporation
```

```
FILE 'WPIX' ENTERED AT 13:20:37 ON 04 JAN 2010
COPYRIGHT (C) 2010 THOMSON REUTERS
PROCESSING COMPLETED FOR L39
PROCESSING COMPLETED FOR L38
L40      8 DUP REM L39 L38 (8 DUPLICATES REMOVED)
          ANSWERS '1-6' FROM FILE ZCAPLUS
          ANSWERS '7-8' FROM FILE MEDLINE
```

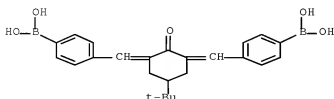
```
=> d ibib abs hitind hitstr L40 1-6; d iall L40 7-8
```

```
L40 ANSWER 1 OF 8 ZCAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 1
ACCESSION NUMBER:      2006:315088 ZCAPLUS Full-text
DOCUMENT NUMBER:      145:290
TITLE:                Anticancer activities of novel chalcone and
                        bis-chalcone derivatives
AUTHOR(S):            Modzelewska, Aneta; Pettit, Catherine; Achanta,
                        Geetha; Davidson, Nancy E.; Huang, Peng; Khan, Saad
                        R.
CORPORATE SOURCE:      Division of Chemical Therapeutics, Sidney Kimmel
                        Comprehensive Cancer Center at Johns Hopkins,
                        Baltimore, MD, 21231, USA
SOURCE:                Bioorganic & Medicinal Chemistry (2006), 14(10),
                        3491-3495
                        CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER:            Elsevier B.V.
DOCUMENT TYPE:         Journal
LANGUAGE:              English
OTHER SOURCE(S):       CASREACT 145:290
GI
```



I

- AB A series of novel chalcones and bis-chalcones containing boronic acid moieties has been synthesized and evaluated for antitumor activity against the human breast cancer MDA-MB-231 (estrogen receptor-neg.) and MCF7 (estrogen receptor-pos.) cell lines and against two normal breast epithelial cell lines, MCF-10A and MCF-12A. These moieties inhibited the growth of the human breast cancer cell lines at low micromolar to nanomolar concns., with five of them showing preferential inhibition of the human breast cancer cell lines. Furthermore, bis-chalcone I exhibited a more potent inhibition of colon cancer cells expressing wild-type p53 than of an isogenic cell line that was p53-null.
- CC 1-3 (Pharmacology)
- IT 19152-38-6P 104169-80-4P 856849-32-6P 888203-72-3P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (anticancer activities of chalcone and bis-chalcone derivs.)
- IT 86293-53-0P 856849-35-9P 888203-68-7P
 888203-69-8P 888203-70-1P 888203-71-2P
 888203-73-4P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (anticancer activities of chalcone and bis-chalcone derivs.)
- IT 856849-32-6P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (anticancer activities of chalcone and bis-chalcone derivs.)
- RN 856849-32-6 ZCAPLUS
- CN Boronic acid, [[5-(1,1-dimethylethyl)-2-oxo-1,3-cyclohexanediyldiene]bis(methyldiylne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



10/596571

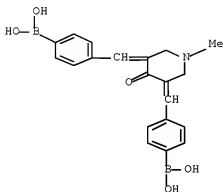
IT 856849-35-9P 888203-68-7P 888203-69-8P
888203-70-1P 888203-71-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(anticancer activities of chalcone and bis-chalcone derivs.)

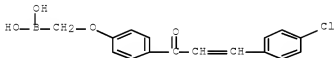
RN 856849-35-9 ZCAPLUS

CN Boronic acid, [(1-methyl-4-oxo-3,5-piperidinediylidene)bis(methylidyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



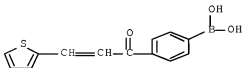
RN 888203-68-7 ZCAPLUS

CN Boronic acid, B-[[4-[3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]phenoxy)methyl]- (CA INDEX NAME)



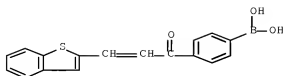
RN 888203-69-8 ZCAPLUS

CN Boronic acid, B-[4-[1-oxo-3-(2-thienyl)-2-propen-1-yl]phenyl]- (CA INDEX NAME)

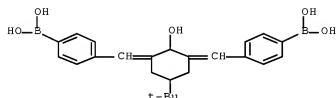


RN 888203-70-1 ZCAPLUS

CN Boronic acid, B-[4-(3-benzo[b]thien-2-yl-1-oxo-2-propen-1-yl)phenyl]- (CA INDEX NAME)



RN 888203-71-2 ZCAPLUS
 CN Boronic acid, [[5-(1,1-dimethylethyl)-2-hydroxy-1,3-cyclohexanediylidene]bis(methyldiylne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 2 OF 8 ZCAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2006:658516 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:262670

TITLE: A boronic-chalcone derivative exhibits potent anticancer activity through inhibition of the proteasome

AUTHOR(S): Achanta, Geetha; Modzelewska, Aneta; Feng, Li; Khan, Saeed R.; Huang, Peng

CORPORATE SOURCE: Department of Molecular Pathology, University of Texas MD Anderson Cancer Center, Houston, TX, USA

SOURCE: Molecular Pharmacology (2006), 70(1), 426-433

CODEN: MOPMA3; ISSN: 0026-895X

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chalcones and their derivs. have been shown to have potent anticancer activity. However, the exact mechanisms of cytotoxic activity remain to be established. In this study, we have evaluated a series of boronic chalcones for their anticancer activity and mechanisms of action. Among the eight chalcone derivs. tested, 3,5-bis-(4-boronic acid-benzylidene)-1-methyl-piperidin-4-one (AM114) exhibited most potent growth inhibitory activity with IC50 values of 1.5 and 0.6 μ M in 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assay and colony formation assay, resp. The cytotoxic activity of AM114 was shown to be associated with the accumulation of p53 and p21 proteins and induction of apoptosis. Mechanistic studies

showed that AM114 treatment inhibited the chymotrypsin-like activity of the 20S proteasome in vitro, leading to a significant accumulation of ubiquitinated p53 and other cellular proteins in whole cells. In vitro studies showed that AM114 did not significantly disrupt the interaction of p53 and murine double minute 2 protein. It is noteworthy that AM114 as a single agent was preferentially toxic to cells with wild-type p53 expression, whereas combination of this compound with ionizing radiation (IR) significantly enhanced the cell-killing activity of IR in both wild-type p53 and p53-null cells. Together, these results indicate that the boronic chalcone derivative AM114 induces significant cytotoxic effect in cancer cells through the inhibition of the cellular proteasome and provide a rationale for the further development of this class of compds. as novel cancer chemotherapeutic agents.

CC 1-6 (Pharmacology)

IT 856849-35-9

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(boronic-chalcone derivative exhibits potent anticancer activity through inhibition of proteasome)

IT 19152-38-6 856849-32-6 888203-68-7

888203-71-2 888203-73-4 906533-53-7 906533-57-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(boronic-chalcone derivative exhibits potent anticancer activity through inhibition of proteasome)

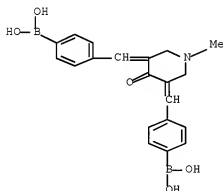
IT 856849-35-9

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(boronic-chalcone derivative exhibits potent anticancer activity through inhibition of proteasome)

RN 856849-35-9 ZCAPLUS

CN Boronic acid, [(1-methyl-4-oxo-3,5-piperidinediylidene)bis(methylidyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



IT 856849-32-6 888203-68-7 888203-71-2

906533-53-7

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

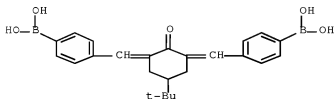
(boronic-chalcone derivative exhibits potent anticancer activity through inhibition of proteasome)

RN 856849-32-6 ZCAPLUS

CN Boronic acid, [(5-(1,1-dimethylethyl)-2-oxo-1,3-

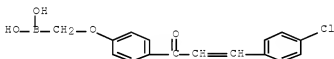
10/596571

cyclohexanediylidene]bis(methyldiyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



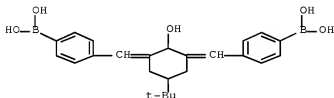
RN 888203-68-7 ZCAPLUS

CN Boronic acid, B-[[4-[3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]phenoxy]methyl]- (CA INDEX NAME)



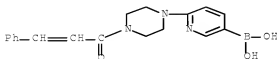
RN 888203-71-2 ZCAPLUS

CN Boronic acid, [[5-(1,1-dimethylethyl)-2-hydroxy-1,3-cyclohexanediylidene]bis(methyldiyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



RN 906533-53-7 ZCAPLUS

CN Boronic acid, B-[6-[4-(1-oxo-3-phenyl-2-propen-1-yl)-1-piperazinyl]-3-pyridinyl]- (CA INDEX NAME)



10/596571

OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS
RECORD (15 CITINGS)
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 3 OF 8 ZCAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2005:612309 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:91012
TITLE: Boronic acid aryl analogs for the treatment of cancer
INVENTOR(S): Khan, Saeed R.
PATENT ASSIGNEE(S): Johns Hopkins University, USA
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063774	A1	20050714	WO 2004-US43114	20041221
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 20080171723	A1	20080717	US 2007-596751	20071018
PRIORITY APPLN. INFO.:			US 2003-531765P	P 20031222
			WO 2004-US43114	W 20041221

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:91012

AB The invention discloses boronic acid aryl derivs. which are useful as antitumor/anticancer agents. The compds., which are inexpensive to synthesize, exhibit unexpectedly good inhibitors of the growth of human breast cancer cells. The invention also discloses the use of the boronic acid aryl derivs. to treat cancer. The invention also provides pharmaceutical compns. comprising the inhibitors of the invention and methods for using the inhibitors and pharmaceutical compns. in the treatment and prevention of cancer.

IC ICM C07F005-02
ICS A61P035-00; A61K031-69

CC 1-6 (Pharmacology)
Section cross-reference(s): 63

ST aryl boronic acid deriv cancer treatment; breast cancer treatment
aryl boronic acid deriv

IT Bone, neoplasm
(Ewing's sarcoma; boronic acid aryl derivs. for treatment of cancer)

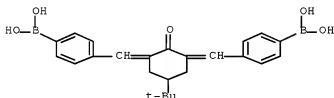
IT Sarcoma
(Ewing's; boronic acid aryl derivs. for treatment of cancer)

IT Sarcoma
(Kaposi's; boronic acid aryl derivs. for treatment of cancer)

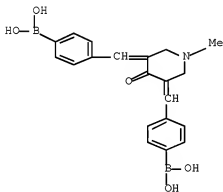
- IT Intestine
(anus, cancer; boronic acid aryl derivs. for treatment of cancer)
- IT Skin, neoplasm
(basal cell carcinoma; boronic acid aryl derivs. for treatment of cancer)
- IT Carcinoma
(basal cell; boronic acid aryl derivs. for treatment of cancer)
- IT Acute lymphocytic leukemia
Acute myeloid leukemia
Antitumor agents
Bladder, neoplasm
Brain, neoplasm
Central nervous system, neoplasm
Esophagus, neoplasm
Eye, neoplasm
Head and Neck, neoplasm
Head and Neck, neoplasm
Human
Kidney, neoplasm
Larynx, neoplasm
Liver, neoplasm
Lung, neoplasm
Lymphoma
Mammary gland, neoplasm
Melanoma
Mouth, neoplasm
Neoplasm
Ovary, neoplasm
Pancreas, neoplasm
Pharynx, neoplasm
Prostate gland, neoplasm
Stomach, neoplasm
Testis, neoplasm
Uterus, neoplasm
(boronic acid aryl derivs. for treatment of cancer)
- IT Mdm2 protein
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(boronic acid aryl derivs. for treatment of cancer)
- IT Uterus, neoplasm
(cervix; boronic acid aryl derivs. for treatment of cancer)
- IT Intestine, neoplasm
(colon; boronic acid aryl derivs. for treatment of cancer)
- IT Neoplasm
Neoplasm
(head and neck; boronic acid aryl derivs. for treatment of cancer)
- IT Carcinoma
(pulmonary small-cell; boronic acid aryl derivs. for treatment of cancer)
- IT Intestine, neoplasm
(rectum; boronic acid aryl derivs. for treatment of cancer)
- IT Lung, neoplasm
(small-cell carcinoma; boronic acid aryl derivs. for treatment of cancer)
- IT Carcinoma

10/596571

(squamous cell; boronic acid aryl derivs. for treatment of cancer)
 IT 856849-32-6 856849-35-9
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (boronic acid aryl derivs. for treatment of cancer)
 IT 856849-32-6 856849-35-9
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (boronic acid aryl derivs. for treatment of cancer)
 RN 856849-32-6 ZCAPLUS
 CN Boronic acid, [[5-(1,1-dimethylethyl)-2-oxo-1,3-cyclohexanediylidene]bis(methyldiyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



RN 856849-35-9 ZCAPLUS
 CN Boronic acid, [(1-methyl-4-oxo-3,5-piperidinediylidene)bis(methyldiyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 4 OF 8 ZCAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 4
 ACCESSION NUMBER: 2003:1006923 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 140:59511
 TITLE: Preparation of boronic chalcone derivatives as anticancer agents

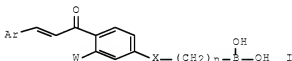
10/596571

INVENTOR(S): Khan, Saeed R.
 PATENT ASSIGNEE(S): Johns Hopkins University, USA
 SOURCE: PCT Int. Appl., 56 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106384	A2	20031224	WO 2003-US18962	20030612
WO 2003106384	A3	20040617		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, BR, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003243594	A1	20031231	AU 2003-243594	20030612
US 20050176988	A1	20050811	US 2005-517781	20050420
US 7514579	B2	20090407		
US 20090227542	A1	20090910	US 2009-403288	20090312
PRIORITY APPLN. INFO.:			US 2002-388255P	P 20020613
			US 2003-44429P	P 20030203
			WO 2003-US18962	W 20030612
			US 2005-517781	A3 20050420

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 140:59511
 GI



AB The present invention relates to novel boronic chalcone derivs. I [Ar = (un)substituted heteroaryl, etc.; W = H, etc.; X = Zn, etc.; n = 0 or any integer; Z = (un)substituted alkylene, etc.] which are useful as antitumor/anticancer agents. The activity of compds. of this invention against the growth of human breast cancer cell lines was demonstrated.

IC ICM C07C

CC 27-10 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 25, 29

IT 562823-84-1P 562823-85-2P 562823-86-3P

562823-87-4P 562823-88-5P 562823-90-9P

562823-91-0P 562823-92-1P 562823-93-2P

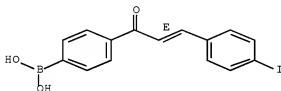
562823-94-3P 562823-95-4P 637347-03-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/596571

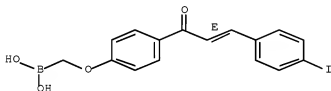
(preparation of boronic chalcone derivs. as anticancer agents)
 IT 562823-84-1P 562823-86-3P 562823-87-4P
 562823-90-9P 562823-91-0P 562823-92-1P
 562823-93-2P 637347-03-6P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (preparation of boronic chalcone derivs. as anticancer agents)
 RN 562823-84-1 ZCAPLUS
 CN Boronic acid, B-[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propen-1-yl]phenyl]-
 (CA INDEX NAME)

Double bond geometry as shown.



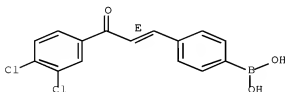
RN 562823-86-3 ZCAPLUS
 CN Boronic acid, [[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propenyl]phenoxy]methyl]-
 (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 562823-87-4 ZCAPLUS
 CN Boronic acid, [4-[(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]-
 (9CI) (CA INDEX NAME)

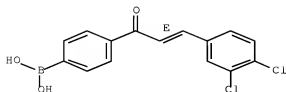
Double bond geometry as shown.



RN 562823-90-9 ZCAPLUS
 CN Boronic acid, [4-[(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]-
 (9CI) (CA INDEX NAME)

10/596571

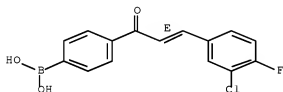
Double bond geometry as shown.



RN 562823-91-0 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-chloro-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

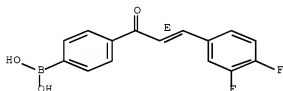
Double bond geometry as shown.



RN 562823-92-1 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-difluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

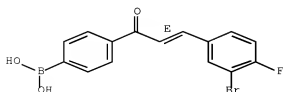
Double bond geometry as shown.



RN 562823-93-2 ZCAPLUS

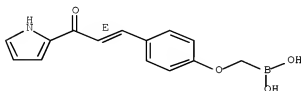
CN Boronic acid, [4-[(2E)-3-(3-bromo-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 637347-03-6 ZCAPLUS
 CN Boronic acid, [[4-[(1E)-3-oxo-3-(1H-pyrrol-2-yl)-1-propenyl]phenoxy)methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
 (5 CITINGS)
 REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 5 OF 8 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:875616 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:387007

TITLE: Template-directed synthesis of multiply mechanically

interlocked molecules under thermodynamic control

Arico, Fabio; Chang, Theresa; Cantrill, Stuart J.;

Khan, Saeed I.; Stoddart, J. Fraser

CORPORATE SOURCE: California NanoSystems Institute and Department of
 Chemistry and Biochemistry, University of California,
 Los Angeles, CA, 90095-1569, USA

SOURCE: Chemistry--A European Journal (2005), 11(16),
 4655-4666

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:387007

AB The template-directed construction of crown-ether-like macrocyclic compds. around secondary dialkylammonium ions (R₂NH₂⁺) has been utilized for the expedient (one-pot) and high-yielding synthesis of a diverse range of mech. interlocked mols. The clipping together of appropriately designed dialdehyde and diamine compds. around R₂NH₂⁺-containing dumbbell-shaped components proceeds through the formation, under thermodyn. control, of imine bonds. The reversible nature of this particular reaction confers the benefits of error-checking and proof-reading, which one usually assoc. with supramol. chemical and strict self-assembly processes, upon these wholly mol. systems. Furthermore, these dynamic covalent syntheses exploit the efficient templating effects that the R₂NH₂⁺ ions exert on the macrocyclization of the matched dialdehyde and diamine fragments, resulting not only in rapid rates of reaction, but also affording near-quant. conversion of starting materials into the desired interlocked products. Once assembled, these dynamic interlocked compds. can be fixed upon reduction of the reversible imine bonds (by using BH₃·THF) to give kinetically stable species, a procedure that can be performed in the same reaction vessel as the initial thermodynamically controlled assembly. Isolation and purification of the mech. interlocked products formed

by using this protocol is relatively facile, as no column chromatog. is required. This article describes the synthesis and characterization of a [2]rotaxane, a [3]rotaxane, a branched [4]rotaxane, a bis [2]rotaxane, and a novel cyclic [4]rotaxane, demonstrating, in incrementally more complex systems, the efficacy of this one-pot strategy for the construction of interlocked mols.

CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
 IT 539-48-0, p-Xylylenediamine 4612-26-4, 1,4-(Phenylene)bis(boronic acid) 5431-44-7, 2,6-Pyridinedicarboxaldehyde 7311-34-4, 3,5-Dimethoxybenzaldehyde 62107-77-1 128184-01-0 256225-29-3 753459-23-3 866783-82-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of rotaxane compds. (multiply mech. interlocked compds.) using template-directed, dynamic chemical synthesis methods under thermodyn. control)
 OS.CITING REF COUNT: 46 THERE ARE 46 CAPLUS RECORDS THAT CITE THIS RECORD (46 CITINGS)
 REFERENCE COUNT: 164 THERE ARE 164 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 6 OF 8 ZCAPLUS COPYRIGHT 2010 ACS ON STN

ACCESSION NUMBER: 2003:410905 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 139:117464

TITLE: Design, Synthesis, and Evaluation of Novel Boronic-Chalcone Derivatives as Antitumor Agents
 AUTHOR(S): Kumar, Srinivas K.; Hager, Erin; Pettit, Catherine; Gurulingappa, Hallur; Davidson, Nancy E.; Khan, Saeed R.

CORPORATE SOURCE: Division of Experimental Therapeutics, Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins, Baltimore, MD, 21231, USA

SOURCE: Journal of Medicinal Chemistry (2003), 46(14), 2813-2815

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:117464

AB A series of boronic-chalcone derivs., e.g. 4-IC6H4CH:CHCOC6H4B(OH)2-4, were synthesized and tested for antitumor activity against human breast cancer cell lines. The results show the boronic-chalcones are more toxic to breast cancer cells compared to normal breast cells than other known chalcones.

CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 1

IT 22563-48-0P 562823-84-1P 562823-86-3P

562823-87-4P 562823-88-5P 562823-89-6P

562823-90-9P 562823-91-0P 562823-92-1P

562823-93-2P 562823-94-3P 562823-95-4P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation)

(design, synthesis, and evaluation of novel boronic-chalcone derivs. as antitumor agents)

IT 562823-84-1P 562823-86-3P 562823-87-4P

562823-89-6P 562823-90-9P 562823-91-0P

562823-92-1P 562823-93-2P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation)

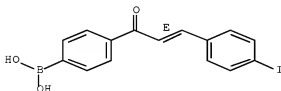
(design, synthesis, and evaluation of novel boronic-chalcone derivs. as antitumor agents)

10/596571

RN 562823-84-1 ZCAPLUS

CN Boronic acid, B-[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propen-1-yl]phenyl]-
(CA INDEX NAME)

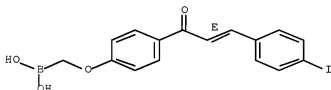
Double bond geometry as shown.



RN 562823-86-3 ZCAPLUS

CN Boronic acid, [[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propenyl]phenoxy]methyl]-
(9CI) (CA INDEX NAME)

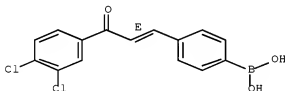
Double bond geometry as shown.



RN 562823-87-4 ZCAPLUS

CN Boronic acid, [4-[(1E)-3-(3,4-dichlorophenyl)-3-oxo-1-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

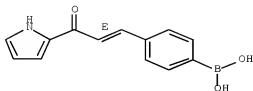


RN 562823-89-6 ZCAPLUS

CN Boronic acid, [4-[(1E)-3-oxo-3-(1H-pyrrol-2-yl)-1-propenyl]phenyl]- (9CI)
(CA INDEX NAME)

Double bond geometry as shown.

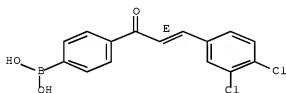
10/596571



RN 562823-90-9 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

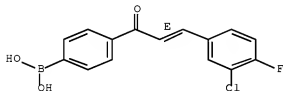
Double bond geometry as shown.



RN 562823-91-0 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-chloro-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

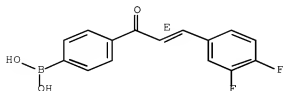
Double bond geometry as shown.



RN 562823-92-1 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-difluorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

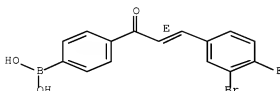


10/596571

RN 562823-93-2 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-bromo-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 87 THERE ARE 87 CAPLUS RECORDS THAT CITE THIS
RECORD (87 CITINGS)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 7 OF 8 MEDLINE on STN
ACCESSION NUMBER: 2009515707 MEDLINE Full-text
DOCUMENT NUMBER: PubMed ID: 19388929
TITLE: Inhibitor of DASH proteases affects expression of adhesion
molecules in osteoclasts and reduces myeloma growth and
bone disease.
AUTHOR: Pennisi Angela; Li Xin; Ling Wen; Khan Sharmin; Gaddy
Dana; Suva Larry J; Barlogie Bart; Shaughnessy John D; Aziz
Nazneen; Yaccoby Shmuel
CORPORATE SOURCE: Myeloma Institute for Research and Therapy, University of
Arkansas for Medical Sciences, Little Rock, AR 72205, USA.
CONTRACT NUMBER: CA-93897 (United States NCI NIH HHS)
R01 CA093897-06 (United States NCI NIH HHS)
SOURCE: British journal of haematology, (2009 Jun) Vol. 145, No. 6,
pp. 775-87. Electronic Publication: 2009-04-08.
Journal code: 0372544. E-ISSN: 1365-2141.
Report No.: NLM-NIHMS145058; NLM-PMC2748971.
PUB. COUNTRY: England; United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
(RESEARCH SUPPORT, N.I.H., EXTRAMURAL)
(RESEARCH SUPPORT, NON-U.S. GOV'T)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200909
ENTRY DATE: Entered STN: 30 Jul 2009
Last Updated on STN: 11 Sep 2009
Entered Medline: 10 Sep 2009

ABSTRACT:
Dipeptidyl peptidase (DPP) IV activity and/or structure homologues (DASH) are
serine proteases implicated in tumourigenesis. We previously found that a DASH
protease, fibroblast activation protein (FAP), was involved in
osteoclast-induced myeloma growth. Here we further demonstrated expression of
various adhesion molecules in osteoclasts cultured alone or cocultured with
myeloma cells, and tested the effects of DASH inhibitor, PT-100, on myeloma
cell growth, bone disease, osteoclast differentiation and activity, and

expression of adhesion molecules in osteoclasts. PT-100 had no direct effects on viability of myeloma cells or mature osteoclasts, but significantly reduced survival of myeloma cells cocultured with osteoclasts. Real-time PCR array for 85 adhesion molecules revealed upregulation of 17 genes in osteoclasts after coculture with myeloma cells. Treatment of myeloma/osteoclast cocultures with PT-100 significantly downregulated 18 of 85 tested genes in osteoclasts, some of which are known to play roles in tumorigenesis and osteoclastogenesis. PT-100 also inhibited osteoclast differentiation and subsequent pit formation. Resorption activity of mature osteoclasts and differentiation of osteoblasts were not affected by PT-100. In primary myelomatous severe combined immunodeficient (SCID)-hu mice PT-100 reduced osteoclast activity, bone resorption and tumour burden. These data demonstrated that DASH proteases are involved in myeloma bone disease and tumour growth.

CONTROLLED TERM: Alkaline Phosphatase: ME, metabolism
Animals
Bone Density: DE, drug effects
Bone Resorption: DT, drug therapy
Bone Resorption: ME, metabolism
*Boronic Acids: TU, therapeutic use
Cell Adhesion Molecules: GE, genetics
*Cell Adhesion Molecules: ME, metabolism
Cell Differentiation: DE, drug effects
Coculture Techniques
*Dipeptides: TU, therapeutic use
*Dipeptidyl Peptidases: AI, antagonists & inhibitors
Gene Expression
Gene Expression Profiling: MT, methods
Humans
Immunoglobulin Light Chains: BL, blood
Immunohistochemistry
Mice
Mice, SCID
*Multiple Myeloma: DT, drug therapy
Multiple Myeloma: ME, metabolism
Multiple Myeloma: PA, pathology
NF-kappa B: ME, metabolism
Oligonucleotide Array Sequence Analysis
Osteoclasts: DE, drug effects
*Osteoclasts: ME, metabolism
Osteoclasts: PA, pathology
Phosphorylation
Tumor Markers, Biological: BL, blood
p38 Mitogen-Activated Protein Kinases: ME, metabolism
CHEMICAL NAME: 0 (Boronic Acids); 0 (Cell Adhesion Molecules); 0 (Dipeptides); 0 (Immunoglobulin Light Chains); 0 (NF-kappa B); 0 (Tumor Markers, Biological); 0 (talabostat); EC 2.7.1.37 (p38 Mitogen-Activated Protein Kinases); EC 3.1.3.1 (Alkaline Phosphatase); EC 3.4.14.- (Dipeptidyl Peptidases)

L40 ANSWER 8 OF 8 MEDLINE on STN
ACCESSION NUMBER: 2009003173 MEDLINE [Full-text](#)
DOCUMENT NUMBER: PubMed ID: 18980173
TITLE: The proteasome inhibitor, bortezomib suppresses primary myeloma and stimulates bone formation in myelomatous and nonmyelomatous bones in vivo.
AUTHOR: Pennisi Angela; Li Xin; Ling Wen; Khan Sharmin; Zangari Maurizio; Yaccoby Shmuel
CORPORATE SOURCE: Myeloma Institute for Research and Therapy, University of Arkansas for Medical Sciences, Little Rock, AR 72205, USA.

10/596571

CONTRACT NUMBER: CA-93897 (United States NCI NIH HHS)
R01 CA093897-01A1 (United States NCI NIH HHS)
R01 CA093897-02 (United States NCI NIH HHS)
R01 CA093897-03 (United States NCI NIH HHS)
R01 CA093897-04 (United States NCI NIH HHS)
R01 CA093897-05A1 (United States NCI NIH HHS)
R01 CA093897-06 (United States NCI NIH HHS)
SOURCE: American journal of hematology, (2009 Jan) Vol. 84, No. 1,
pp. 6-14.
Journal code: 7610369. E-ISSN: 1096-8652.
Report No.: NLM-NIHMS78924; NLM-PMC2612734.
COMMENT: Comment in: Am J Hematol. 2009 Jan;84(1):1-2. PubMed ID:
19030185
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
(RESEARCH SUPPORT, N.I.H., EXTRAMURAL)
(RESEARCH SUPPORT, NON-U.S. GOV'T)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200901
ENTRY DATE: Entered STN: 2 Jan 2009
Last Updated on STN: 29 Jan 2009
Entered Medline: 28 Jan 2009

ABSTRACT:

Multiple myeloma (MM), a hematologic malignancy of terminally differentiated plasma cells is closely associated with induction of osteolytic bone disease, induced by stimulation of osteoclastogenesis and suppression of osteoblastogenesis. The ubiquitin-proteasome pathway regulates differentiation of bone cells and MM cell growth. The proteasome inhibitor, bortezomib, is a clinical potent antimyeloma agent. The main goal of this study was to investigate the effect of bortezomib on myeloma-induced bone resorption and tumor growth in SCID-rab mice engrafted with MM cells from 16 patients. Antimyeloma response of bortezomib, which was evident in >50% of 16 experiments and resembled clinical response, was associated with significant increased bone mineral density (BMD) and osteoblast numbers, and reduced osteoclast numbers in myelomatous bones. This bone anabolic effect, which was also visualized on X-ray radiographs and confirmed by static and dynamic histomorphometric analyses, was unique to bortezomib and was not observed in hosts responding to melphalan, a chemotherapeutic drug widely used to treat MM. Bortezomib also increased BMD and osteoblasts number and reduced osteoclasts number in nonmyelomatous implanted bones. In vitro bortezomib directly suppressed human osteoclast formation and promoted maturation of osteoblasts. We conclude that bortezomib promotes bone formation in myelomatous and nonmyelomatous bones by simultaneously inhibiting osteoclastogenesis and stimulating osteoblastogenesis. As clinical and experimental studies indicate that bone disease is both a consequence and necessity of MM progression our results suggest and that bortezomib's effects on bone remodeling contribute to the antimyeloma efficacy of this drug.

CONTROLLED TERM: Animals
Bone Density: DE, drug effects
Bone Density Conservation Agents: PD, pharmacology
*Bone Development: DE, drug effects
*Boronic Acids: PD, pharmacology
Disease Models, Animal
Humans
Mice
Multiple Myeloma: CO, complications
*Multiple Myeloma: DT, drug therapy
Osteoblasts: DE, drug effects
Osteoclasts: DE, drug effects

10/596571

*Osteolysis: DT, drug therapy

Osteolysis: ET, etiology

*Protease Inhibitors: PD, pharmacology

*Pyrazines: PD, pharmacology

Rabbits

CHEMICAL NAME:

0 (Bone Density Conservation Agents); 0 (Boronic
Acids); 0 (Protease Inhibitors); 0 (Pyrazines); 0
(bortezomib)

=> file registry

FILE 'REGISTRY' ENTERED AT 13:21:57 ON 04 JAN 2010
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0
 DICTIONARY FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

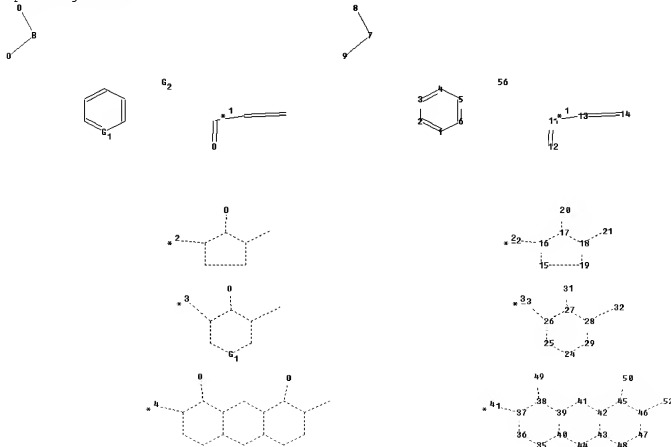
TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

Uploading L3.str



10/596571

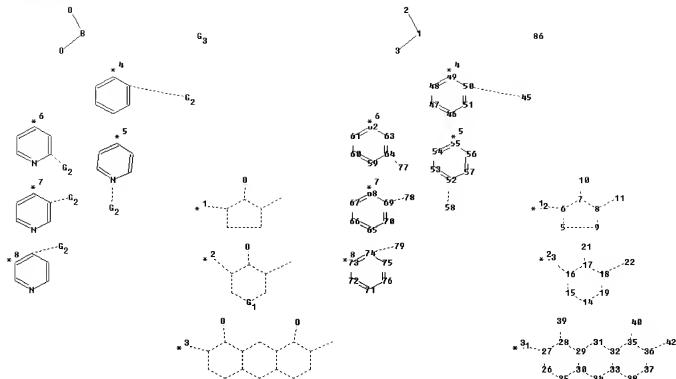
```
chain nodes :
11 12 13 14 20 21 22 23 31 32 49 50 51 52 56
ring nodes :
1 2 3 4 5 6 15 16 17 18 19 24 25 26 27 28 29 35 36 37 38 39
40 41 42 43 44 45 46 47 48
ring/chain nodes :
7 8 9
chain bonds :
11-12 11-13 13-14 16-22 17-20 18-21 23-26 27-31 28-32 37-51 38-49 45-50
46-52
ring/chain bonds :
7-8 7-9
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-19 16-17 17-18 18-19 24-25 24-29 25-
26
26-27 27-28 28-29 35-36 35-40 36-37 37-38 38-39 39-40 39-41 40-44 41-42
42-43 42-45
43-44 43-48 45-46 46-47 47-48
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 11-12 11-13 13-14 15-16 15-19 16-17
16-22 17-18 17-20 18-19 18-21 23-26 24-25 24-29 25-26 26-27 27-28 27-31
28-29 28-32
35-36 35-40 36-37 37-38 37-51 38-39 38-49 39-40 39-41 40-44 41-42 42-43
42-45 43-44 43-48
45-46 45-50 46-47 46-52 47-48
```

G1:C,N

G2:[*1],[*2],[*3],[*4]

```
Connectivity :
15:2 E exact RC ring/chain 16:3 E exact RC ring/chain 17:3 E exact RC ring/chain
18:3 E exact RC ring/chain 19:2 E exact RC ring/chain 20:1 E exact RC ring/chain
21:2 X maximum
RC ring/chain 22:2 E exact RC ring/chain 23:2 E exact RC ring/chain 25:2 E exact
RC ring/chain
26:3 E exact RC ring/chain 27:3 E exact RC ring/chain 28:3 E exact RC ring/chain
29:2 E exact
RC ring/chain 31:1 E exact RC ring/chain 32:2 X maximum RC ring/chain 38:3 E
exact RC ring/chain
45:3 E exact RC ring/chain 46:3 E exact RC ring/chain 49:1 E exact RC ring/chain
50:1 E exact
RC ring/chain 51:2 E exact RC ring/chain 52:2 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS
22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:CLASS
32:CLASS 35:Atom
36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom
47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 56:CLASS
```

Uploading L11.str



chain nodes :

10 11 12 13 21 22 39 40 41 42 45 58 77 78 79 86

ring nodes :

5 6 7 8 9 14 15 16 17 18 19 25 26 27 28 29 30 31 32 33 34 35
 36 37 38 46 47 48 49 50 51 52 53 54 55 56 57 59 60 61 62 63 64
 65 66 67 68
 69 70 71 72 73 74 75 76

ring/chain nodes :

1 2 3

chain bonds :

6-12 7-10 8-11 13-16 17-21 18-22 27-41 28-39 35-40 36-42 45-50 52-58
 64-77 69-78 74-79

ring/chain bonds :

1-2 1-3

ring bonds :

5-6 5-9 6-7 7-8 8-9 14-15 14-19 15-16 16-17 17-18 18-19 25-26 25-30
 26-27 27-28 28-29 29-30 29-31 30-34 31-32 32-33 32-35 33-34 33-38 35-36
 36-37 37-38 46-47
 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 56-57 59-60
 59-64 60-61
 61-62 62-63 63-64 65-66 65-70 66-67 67-68 68-69 69-70 71-72 71-76 72-73
 73-74 74-75
 75-76

exact/norm bonds :

1-2 1-3 5-6 5-9 6-7 6-12 7-8 7-10 8-9 8-11 13-16 14-15 14-19 15-16
 16-17 17-18 17-21 18-19 18-22 25-26 25-30 26-27 27-28 27-41 28-29 28-39
 29-30 29-31 30-34
 31-32 32-33 32-35 33-34 33-38 35-36 35-40 36-37 36-42 37-38 45-50 52-58
 64-77 69-78
 74-79

normalized bonds :

46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 56-57
 59-60 59-64 60-61 61-62 62-63 63-64 65-66 65-70 66-67 67-68 68-69 69-70

10/596571

71-72 71-76

72-73 73-74 74-75 75-76

G1:C,N

G2:[*1],[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8]

Match level :

1:CLASS 2:CLASS 3:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS
12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS
22:CLASS
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom
34:Atom 35:Atom
36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:CLASS
46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom
58:CLASS 59:CLASS
60:CLASS 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom
69:Atom
70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:CLASS 78:CLASS
79:CLASS 86:CLASS

=> file zcaplus

FILE 'ZCAPLUS' ENTERED AT 13:22:00 ON 04 JAN 2010

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 4 Jan 2010 VOL 152 ISS 2

FILE LAST UPDATED: 3 Jan 2010 (20100103/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate

10/596571

substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L14

L13 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

L7 995 SEA FILE=REGISTRY SSS FUL L3

L11 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L13 4 SEA FILE=REGISTRY SUB=L7 SSS FUL L11

L14 4 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L13

=> d ibib abs hitstr L14 1-4

L14 ANSWER 1 OF 4 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2006:658516 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:262670

TITLE: A boronic-chalcone derivative exhibits potent anticancer activity through inhibition of the proteasome

AUTHOR(S): Achanta, Geetha; Modzelewska, Aneta; Feng, Li; Khan, Saeed R.; Huang, Peng

CORPORATE SOURCE: Department of Molecular Pathology, University of Texas MD Anderson Cancer Center, Houston, TX, USA

SOURCE: Molecular Pharmacology (2006), 70(1), 426-433
CODEN: MOPMA3; ISSN: 0026-895X

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chalcones and their derivs. have been shown to have potent anticancer activity. However, the exact mechanisms of cytotoxic activity remain to be established. In this study, we have evaluated a series of boronic chalcones for their anticancer activity and mechanisms of action. Among the eight chalcone derivs. tested, 3,5-bis-(4-boronic acid-benzylidene)-1-methyl-piperidin-4-one (AM114) exhibited most potent growth inhibitory activity with IC50 values of 1.5 and 0.6 μ M in 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assay and colony formation assay, resp. The cytotoxic activity of AM114 was shown to be associated with the accumulation of p53 and p21 proteins and induction of apoptosis. Mechanistic studies showed that AM114 treatment inhibited the chymotrypsin-like activity of the 20S proteasome in vitro, leading to a significant accumulation of ubiquitinated p53 and other cellular proteins in whole cells. In vitro studies showed that AM114 did not significantly disrupt the interaction of p53 and murine double minute 2 protein. It is noteworthy that AM114 as a single agent was preferentially toxic to cells with wild-type p53 expression, whereas combination of this compound with ionizing radiation (IR) significantly enhanced the cell-killing activity of IR in both wild-type p53 and p53-null cells. Together, these results indicate that the boronic chalcone derivative AM114 induces significant cytotoxic effect in cancer cells through the inhibition of the cellular proteasome and provide a rationale for the further development of this class of compds. as novel cancer chemotherapeutic agents.

IT 856849-35-9

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU

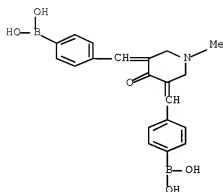
10/596571

(Therapeutic use); BIOL (Biological study); USES (Uses)

(boronic-chalcone derivative exhibits potent anticancer activity through inhibition of proteasome)

RN 856849-35-9 ZCAPLUS

CN Boronic acid, [(1-methyl-4-oxo-3,5-piperidinediylidene)bis(methyldiyn-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



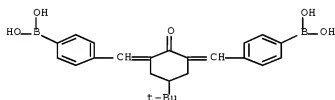
IT 856849-32-6 888203-71-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(boronic-chalcone derivative exhibits potent anticancer activity through inhibition of proteasome)

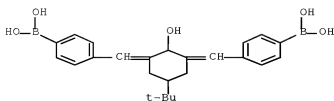
RN 856849-32-6 ZCAPLUS

CN Boronic acid, [[5-(1,1-dimethylethyl)-2-oxo-1,3-cyclohexanediylidene]bis(methyldiyn-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



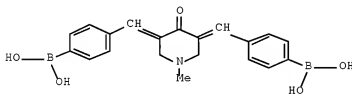
RN 888203-71-2 ZCAPLUS

CN Boronic acid, [[5-(1,1-dimethylethyl)-2-hydroxy-1,3-cyclohexanediylidene]bis(methyldiyn-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
 REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2010 ACS ON STN
 ACCESSION NUMBER: 2006:315088 ZCAPLUS Full-text
 DOCUMENT NUMBER: 145:290
 TITLE: Anticancer activities of novel chalcone and bis-chalcone derivatives
 AUTHOR(S): Modzelewska, Aneta; Pettit, Catherine; Achanta, Geetha; Davidson, Nancy E.; Huang, Peng; Khan, Saeed R.
 CORPORATE SOURCE: Division of Chemical Therapeutics, Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins, Baltimore, MD, 21231, USA
 SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(10), 3491-3495
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:290
 GI



I

AB A series of novel chalcones and bis-chalcones containing boronic acid moieties has been synthesized and evaluated for antitumor activity against the human breast cancer MDA-MB-231 (estrogen receptor-neg.) and MCF7 (estrogen receptor-pos.) cell lines and against two normal breast epithelial cell lines, MCF-10A and MCF-12A. These mols. inhibited the growth of the human breast cancer cell lines at low micromolar to nanomolar concns., with five of them showing preferential inhibition of the human breast cancer cell lines. Furthermore,

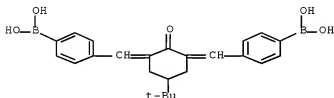
10/596571

bis-chalcone I exhibited a more potent inhibition of colon cancer cells expressing wild-type p53 than of an isogenic cell line that was p53-null.

IT 856849-32-6P
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (anticancer activities of chalcone and bis-chalcone derivs.)

RN 856849-32-6 ZCAPLUS

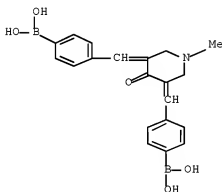
CN Boronic acid, [[5-(1,1-dimethylethyl)-2-oxo-1,3-cyclohexanediylidene]bis(methyldiyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



IT 856849-35-9P 888203-71-2P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (anticancer activities of chalcone and bis-chalcone derivs.)

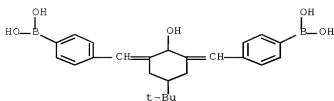
RN 856849-35-9 ZCAPLUS

CN Boronic acid, [[(1-methyl-4-oxo-3,5-piperidinediylidene)bis(methyldiyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



RN 888203-71-2 ZCAPLUS

CN Boronic acid, [[5-(1,1-dimethylethyl)-2-hydroxy-1,3-cyclohexanediylidene]bis(methyldiyne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 4 ZCAPLUS COPYRIGHT 2010 ACS ON STN
 ACCESSION NUMBER: 2005:612309 ZCAPLUS Full-text
 DOCUMENT NUMBER: 143:91012
 TITLE: Boronic acid aryl analogs for the treatment of cancer
 INVENTOR(S): Khan, Saeed R.
 PATENT ASSIGNEE(S): Johns Hopkins University, USA
 SOURCE: PCT Int. Appl., 51 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063774	A1	20050714	WO 2004-US43114	20041221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20080171723	A1	20080717	US 2007-596751	20071018
PRIORITY APPLN. INFO.:			US 2003-531765P	P 20031222
			WO 2004-US43114	W 20041221

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 143:91012

AB The invention discloses boronic acid aryl derivs. which are useful as antitumor/anticancer agents. The compds., which are inexpensive to synthesize, exhibit unexpectedly good inhibitors of the growth of human breast cancer cells. The invention also discloses the use of the boronic acid aryl derivs. to treat cancer. The invention also provides pharmaceutical compns. comprising the inhibitors of the invention and methods for using the inhibitors and pharmaceutical compns. in the treatment and prevention of cancer.

IT 856849-32-6 856849-35-9

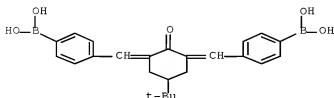
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

10/596571

(boronic acid aryl derivs. for treatment of cancer)

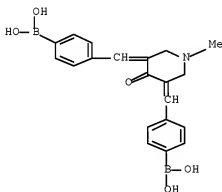
RN 856849-32-6 ZCAPLUS

CN Boronic acid, [[5-(1,1-dimethylethyl)-2-oxo-1,3-cyclohexanediylidene]bis(methyldiylne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



RN 856849-35-9 ZCAPLUS

CN Boronic acid, [(1-methyl-4-oxo-3,5-piperidinediylidene)bis(methyldiylne-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 4 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1986:538657 ZCAPLUS Full-text

DOCUMENT NUMBER: 105:138657

ORIGINAL REFERENCE NO.: 105:22303a,22306a

TITLE: Silicon carbide base sintered material containing boron as a sintering assistant

INVENTOR(S): Saikai, Mikio; Naka, Masaru

PATENT ASSIGNEE(S): Nissan Motor Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 28 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
EP 189181	A2	19860730	EP 1986-100796	19860122
EP 189181	A3	19861230		
R: DE, FR, GB				
JP 61168568	A	19860730	JP 1985-9180	19850123
PRIORITY APPLN. INFO.:			JP 1985-9180	A 19850123

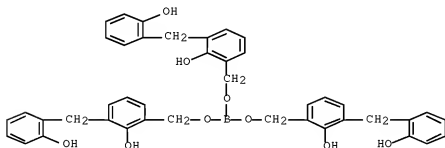
AB In the manufacture of SiC ceramics with B as a sintering aid, an organic compound from the reaction of a B compound and a resol or novolak phenolic resin is used in place of elemental B. The starting B compound is, e.g., H3BO3, BC13, or Et2BOH, and the sintering aid is, e.g., a boric acid ester. A mixture of SiC 100 and organic B-resin compound 2-10 weight parts is compacted or molded, heated to decompose the B compound, and fired at 1800-2200° to give sintered SiC. Agglomeration of the B in the sintered material is prevented to give uniform sintering and high, reliable mech. strength. Thus, H3BO3 1.5 and a resol phenolic ester 5 g reacted to form (o-HOC6H4CH2C6H3(o-OH)CH2O)3B (I), which was dissolved in 250 mL dioxane and mixed with SiC powder 93.5 g. The slurry was ball-milled, freeze-dried, cold-pressed at 2000 kg/cm2, heated to 900° to decompose and carbonize the I, and fired at 2050° under 10-3 to 10-4 mmHg vacuum for 30 min. The resulting ceramic piece had d. 3.11 g/cm3 (97.2% theor. d.), average flexural strength (30 samples) 97.8 kg/mm2, and Weibull coefficient 15.3, vs. 3.08, 75.6, and 5.4 for a similar piece manufactured with elemental B as sintering aid.

IT 104503-70-QP

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as sintering aid for silicon carbide ceramics)

RN 104503-70-0 ZCAPLUS

CN Benzenemethanol, 2-hydroxy-3-[(2-hydroxyphenyl)methyl]-,
 α,α',α'' -triester with boric acid (H3BO3) (9CI) (CA
INDEX NAME)



=> file registry

FILE 'REGISTRY' ENTERED AT 13:22:35 ON 04 JAN 2010
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0
 DICTIONARY FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

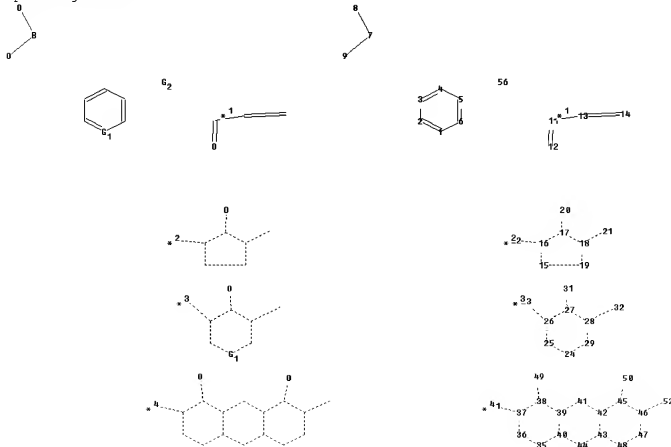
TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

Uploading L3.str



10/596571

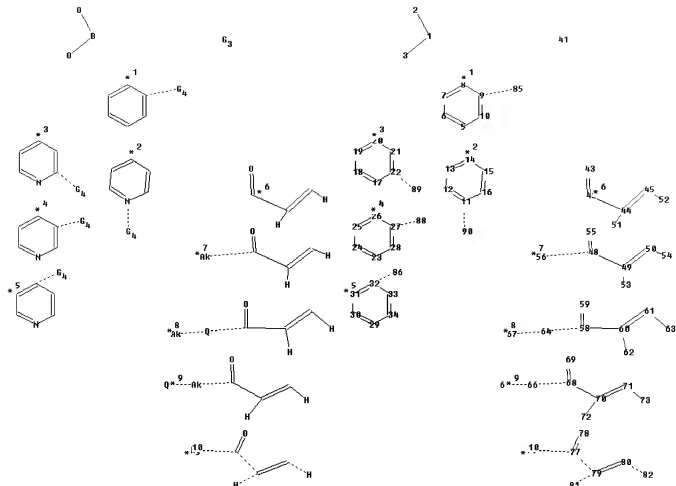
```
chain nodes :
11 12 13 14 20 21 22 23 31 32 49 50 51 52 56
ring nodes :
1 2 3 4 5 6 15 16 17 18 19 24 25 26 27 28 29 35 36 37 38 39
40 41 42 43 44 45 46 47 48
ring/chain nodes :
7 8 9
chain bonds :
11-12 11-13 13-14 16-22 17-20 18-21 23-26 27-31 28-32 37-51 38-49 45-50
46-52
ring/chain bonds :
7-8 7-9
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-19 16-17 17-18 18-19 24-25 24-29 25-
26
26-27 27-28 28-29 35-36 35-40 36-37 37-38 38-39 39-40 39-41 40-44 41-42
42-43 42-45
43-44 43-48 45-46 46-47 47-48
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 11-12 11-13 13-14 15-16 15-19 16-17
16-22 17-18 17-20 18-19 18-21 23-26 24-25 24-29 25-26 26-27 27-28 27-31
28-29 28-32
35-36 35-40 36-37 37-38 37-51 38-39 38-49 39-40 39-41 40-44 41-42 42-43
42-45 43-44 43-48
45-46 45-50 46-47 46-52 47-48
```

G1:C,N

G2:[*1],[*2],[*3],[*4]

```
Connectivity :
15:2 E exact RC ring/chain 16:3 E exact RC ring/chain 17:3 E exact RC ring/chain
18:3 E exact RC ring/chain 19:2 E exact RC ring/chain 20:1 E exact RC ring/chain
21:2 X maximum
RC ring/chain 22:2 E exact RC ring/chain 23:2 E exact RC ring/chain 25:2 E exact
RC ring/chain
26:3 E exact RC ring/chain 27:3 E exact RC ring/chain 28:3 E exact RC ring/chain
29:2 E exact
RC ring/chain 31:1 E exact RC ring/chain 32:2 X maximum RC ring/chain 38:3 E
exact RC ring/chain
45:3 E exact RC ring/chain 46:3 E exact RC ring/chain 49:1 E exact RC ring/chain
50:1 E exact
RC ring/chain 51:2 E exact RC ring/chain 52:2 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS
21:CLASS
22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:CLASS
32:CLASS 35:Atom
36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom
47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 56:CLASS
```

Uploading L15.str



chain nodes :

41 42 43 44 45 48 49 50 51 52 53 54 55 56 58 59 60 61 62 63 64
65 66 67 68 69 70 71 72 73 76 77 78 79 80 81 82 85 86 88 89 90

ring nodes :

5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
27 28 29 30 31 32 33 34

ring/chain nodes :

1-2 3

chain bonds :

9-85 11-90 22-89 27-88 32-86 42-43 42-44 44-45 44-51 45-52 48-49 48-55
48-56 49-50 49-53 50-54 58-59 58-60 58-64 60-61 60-62 61-63 64-67 65-66
66-68 68-69
68-70 70-71 70-72 71-73 76-77 77-78 77-79 79-80 79-81 80-82

ring/chain bonds :

1-2 1-3

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-18
17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 29-30
29-34 30-31 31-32
32-33 33-34

exact/norm bonds :

1-2 1-3 9-85 11-90 22-89 27-88 32-86 42-43 48-55 48-56 58-59 58-64 64-67

65-66 66-68 68-69 76-77 77-78 77-79 79-81 80-82

exact bonds :

42-44 44-45 44-51 45-52 48-49 49-50 49-53 50-54 58-60 60-61 60-62 61-63

10/596571

68-70 70-71 70-72 71-73 79-80

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-18
17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 29-30
29-34 30-31 31-32
32-33 33-34

G1:C,N

G3:[*1],[*2],[*3],[*4],[*5]

G4:[*6],[*7],[*8],[*9],[*10]

Connectivity :

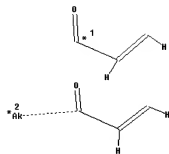
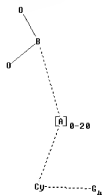
45:2 X maximum RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom 20:Atom
21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom
34:Atom 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 48:CLASS 49:CLASS
50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 58:CLASS 59:CLASS 60:CLASS
61:CLASS 62:CLASS
63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS
71:CLASS 72:CLASS
73:CLASS 76:Atom 77:CLASS 78:CLASS 79:CLASS 80:CLASS 81:CLASS 82:CLASS
85:CLASS 86:CLASS
88:CLASS 89:CLASS 90:CLASS

Uploading L18.str

10/596571



10/596571

G1:C,N

G4:[*1],[*2],[*3],[*4],[*5]

Connectivity :

8:2 X maximum RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 11:CLASS 12:CLASS

13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS

22:CLASS 23:CLASS

24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

32:CLASS 33:CLASS

34:CLASS 35:CLASS 36:CLASS 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS

44:CLASS 45:CLASS

48:Atom 49:CLASS 51:CLASS

Generic attributes :

48:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 48: Limited

C,C6

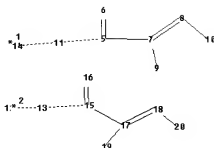
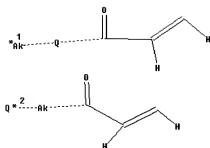
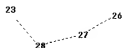
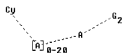
N,N0-1

O,O0

S,S0

Uploading L22.str

10/596571



```

chain nodes :
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 23 26 27 28
ring/chain nodes :
1 2 3
chain bonds :
5-6 5-7 5-11 7-8 7-9 8-10 11-14 12-13 13-15 15-16 15-17 17-18 17-19
18-20 23-28 26-27 27-28
ring/chain bonds :
1-2 1-3
exact/norm bonds :
1-2 1-3 5-6 5-11 11-14 12-13 13-15 15-16 23-28 26-27 27-28
exact bonds :
5-7 7-8 7-9 8-10 15-17 17-18 17-19 18-20

```

G1:C,N

G2:[*1],[*2]

```

Match level :
1:CLASS 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS
23:Atom 26:CLASS 27:CLASS 28:CLASS

```

10/596571

Generic attributes :

23:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 23: Limited

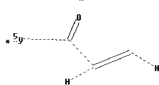
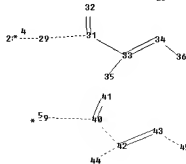
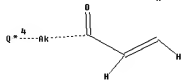
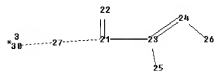
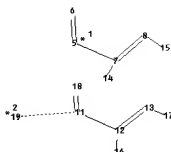
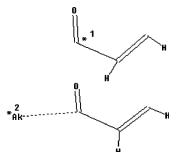
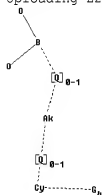
C,C6

N,N0-1

O,O0

S,S0

Uploading L29.str



chain nodes :

10/596571

```
5  6  7  8  11 12 13 14 15 16 17 18 19 21 22 23 24 25 26 27 28 29
30 31 32 33 34 35 36 39 40 41 42 43 44 45 48 49 51 52 55
ring/chain nodes :
1  2  3
chain bonds :
1-52  5-6  5-7  7-8  7-14  8-15  11-12  11-18  11-19  12-13  12-16  13-17  21-22
21-23  21-27  23-24  23-25  24-26  27-30  28-29  29-31  31-32  31-33  33-34  33-35
34-36  39-40
40-41  40-42  42-43  42-44  43-45  48-49  48-55  51-52  51-55
ring/chain bonds :
1-2  1-3
exact/norm bonds :
1-2  1-3  1-52  5-6  11-18  11-19  21-22  21-27  27-30  28-29  29-31  31-32  39-40
40-41  40-42  42-44  43-45  48-49  48-55  51-52  51-55
exact bonds :
5-7  7-8  7-14  8-15  11-12  12-13  12-16  13-17  21-23  23-24  23-25  24-26  31-33
33-34  33-35  34-36  42-43
```

G1:C,N

G4:[*1],[*2],[*3],[*4],[*5]

```
Connectivity :
8:2 X maximum RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS
22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS
34:CLASS 35:CLASS 36:CLASS 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS
44:CLASS 45:CLASS
48:Atom 49:CLASS 51:CLASS 52:CLASS 55:CLASS
Generic attributes :
48:
Saturation      : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
```

```
Element Count :
Node 48: Limited
C,C6
N,N0-1
O,O0
S,S0
```

```
=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 13:22:37 ON 04 JAN 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)
```

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 4 Jan 2010 VOL 152 ISS 2
 FILE LAST UPDATED: 3 Jan 2010 (20100103/ED)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

ZCPlus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L21

L3 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

L7 995 SEA FILE=REGISTRY SSS FUL L3

L15 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

L17 58 SEA FILE=REGISTRY SUB=L7 SSS FUL L15

L18 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

L20 20 SEA FILE=REGISTRY SUB=L17 SSS FUL L18

L21 20 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L20

=> d stat que L26

L3 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

L7 995 SEA FILE=REGISTRY SSS FUL L3

L22 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L24 75 SEA FILE=REGISTRY SUB=L7 SSS FUL L22

L26 15 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L24

10/596571

=> d stat que L33
L3 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

L7 995 SEA FILE=REGISTRY SSS FUL L3
L29 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

L31 2 SEA FILE=REGISTRY SUB=L7 SSS FUL L29
L33 5 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L31

=> s L21 or L26 or L33
L41 34 L21 OR L26 OR L33

=> d ibib abs hitstr L41 1-34

L41 ANSWER 1 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:1339654 ZCAPLUS Full-text

DOCUMENT NUMBER: 151:564335

TITLE: Pharmacophore Modeling for Qualitative Prediction of
Antiestrogenic Activity

AUTHOR(S): Brogi, Simone; Kladi, Maria; Vagias, Constantinos;
Papazafiri, Panagiota; Roussis, Vassilios; Tafi,
Andrea

CORPORATE SOURCE: Dipartimento Farmaco Chimico Tecnologico, Universita
degli Studi di Siena, Siena, I-53100, Italy

SOURCE: Journal of Chemical Information and Modeling (2009),
49(11), 2489-2497

CODEN: JCISD8; ISSN: 1549-9596

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A ligand-based pharmacophore approach for the prediction of antiestrogenic activity to be used as an in silico screening tool for bioactive compds. including natural products was developed using Catalyst HypoGen. The generated pharmacophore hypothesis (HYPO-7) consisted of five features, namely, one hydrophobic (HY1), two hydrophobic aromatic (HY2), one hydrogen-bond acceptor (HBA), and one hydrogen-bond donor (HBD). HYPO-7 successfully predicted the lack of cytotoxicity of a number of new metabolites isolated from the red alga Laurencia glandulifera. Furthermore, a screening of the Asinex Gold Collection database was performed by coupling HYPO-7 with a docking filtration, which resulted in a restricted set of 12 new scaffolds to be investigated as potential SERMs. The inhibitory activity of these compds. was evaluated in vitro using MCF7 human breast adenocarcinoma cell line. Ten out of the twelve compds. exhibited inhibitory activity with IC50 values between 26 and 188 µM. This result shows that application of HYPO-7 could assist in the selection of potentially active compds., thus expediting the hit discovery process.

IT 562823-90-9 562823-91-0 562823-92-1

562823-93-2 1197188-80-9

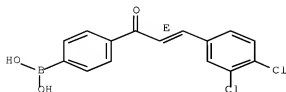
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(pharmacophore modeling for qual. prediction of antiestrogenic
activity)

RN 562823-90-9 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

10/596571

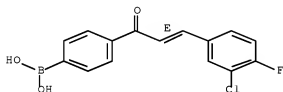
Double bond geometry as shown.



RN 562823-91-0 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-chloro-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

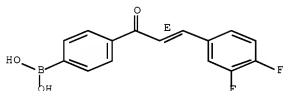
Double bond geometry as shown.



RN 562823-92-1 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-difluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

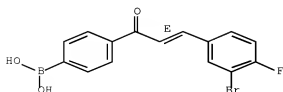
Double bond geometry as shown.



RN 562823-93-2 ZCAPLUS

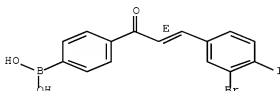
CN Boronic acid, [4-[(2E)-3-(3-bromo-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 1197188-80-9 ZCAPLUS
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 2 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:480379 ZCAPLUS Full-text

DOCUMENT NUMBER: 151:48488

TITLE: Chalcones in cancer: understanding their role in terms of QSAR

AUTHOR(S): Katsori, A.-M.; Hadjipavlou-Litina, D.

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, School of Pharmacy, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece

SOURCE: Current Medicinal Chemistry (2009), 16(9), 1062-1081

CODEN: CMCHE7; ISSN: 0929-8673

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chalcones are a group of plant-derived polyphenolic compds. belonging to the flavonoids family and possess a wide variety of cytoprotective and modulatory functions. The results showed that chalcones inhibit the proliferation of MCF-7 and MDA-MB-231 by inducing apoptosis and blocking cell cycle progression in the G2/M phase. Immunoblot assay showed that chalcones significantly decreased the expression of cyclin B1, cyclin A and Cdc2 protein, as well as increased the expression of p21 and p27 in a p53-independent manner, contributing to cell cycle arrest. In this research we tried to review the anticancer effect of chalcones derivs., and to evaluate new QSARs which will help in the understanding of the role of chalcones and of their analogs on cancer. Simultaneously a comparative study will be presented. Our QSAR results reveal that in almost all cases, the clog P parameter plays an important part in the QSAR relationships (linear or bilinear model). In some cases the steric factors such as the CMR or the substituents MR (linear) are important. Electronic effects are comparatively unimportant. The study shows that log P as calculated from the Clog P program is suitable for this form of QSAR study.

IT 562823-84-1 562823-86-3 562823-90-9

562823-91-0 562823-92-1 562823-93-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(chalcones role in cancer in terms of QSAR)

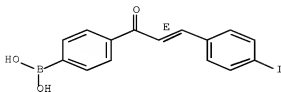
RN 562823-84-1 ZCAPLUS

CN Boronic acid, B-[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propen-1-yl]phenyl]-

10/596571

(CA INDEX NAME)

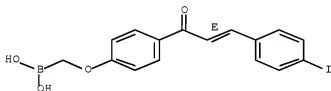
Double bond geometry as shown.



RN 562823-86-3 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propenyl]phenoxy]methyl]-
(9CI) (CA INDEX NAME)

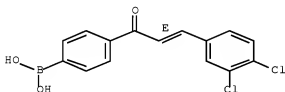
Double bond geometry as shown.



RN 562823-90-9 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

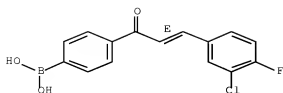


RN 562823-91-0 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-chloro-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

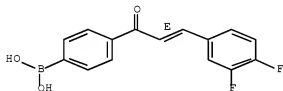
Double bond geometry as shown.

10/596571



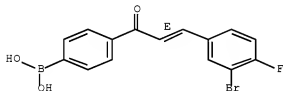
RN 562823-92-1 ZCAPLUS
CN Boronic acid, [4-[(2E)-3-(3,4-difluorophenyl)-1-oxo-2-propenyl]phenyl]-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 562823-93-2 ZCAPLUS
CN Boronic acid, [4-[(2E)-3-(3-bromo-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 3 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:419880 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 151:33269
TITLE: No-carrier-added radiohalogenations utilizing organoboranes: The synthesis of iodine-123 labeled curcumin
AUTHOR(S): Kabalka, George W.; Yao, Min-Liang
CORPORATE SOURCE: Departments of Chemistry and Radiology, The University of Tennessee, Knoxville, TN, 37996-1600, USA
SOURCE: Journal of Organometallic Chemistry (2009), 694(11), 1638-1641
CODEN: JORCAI; ISSN: 0022-328X

10/596571

PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

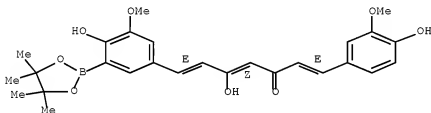
AB The use of organoborane intermediates for radiohalogenations is briefly reviewed. The synthesis of an iodine-123 labeled curcumin derivative using a newly developed radio-iodination technique is reported.

IT 1159575-52-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of iodine-123 labeled curcumin using organoborane intermediates)

RN 1159575-52-6 ZCAPLUS

CN 1,4,6-Heptatrien-3-one, 5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-7-[4-hydroxy-3-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-, (1E,4Z,6E)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 4 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:299944 ZCAPLUS Full-text

DOCUMENT NUMBER: 150:424180

TITLE: Multiresponsive Hybrid Microgels and Hollow Capsules with a Layered Structure

AUTHOR(S): Lapeyre, Veronique; Renaudie, Natacha; Dechezelles, Jean-Francois; Saadaoui, Hassan; Ravaine, Serge; Ravaine, Valerie

CORPORATE SOURCE: Institut des Sciences Moleculaires, Universite Bordeaux, Pessac, 33607, Fr.

SOURCE: Langmuir (2009), 25(8), 4659-4667
CODEN: LANGD5; ISSN: 0743-7463

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Various stimuli-responsive composite particles with a high control of their internal structure and their corresponding hollow capsules are synthesized and characterized by photon correlation spectroscopy, TEM, and AFM. Core-shell particles with a silica core and a thermoresponsive shell are obtained by polymerization of N-isopropylacrylamide (NIPAM) in the presence of silica seeds grafted with a high d. of γ -methacryloxypropyltrimethoxysilane (MPS). The influence of the synthesis conditions is studied. The shell thickness increases when the monomer concentration increases in a limited range where uniform composite particles with a single core are obtained. At constant monomer concentration, the shell thickness does not depend on the size of the silica seeds, but the presence of free unbound microgels is observed when the

silica surface area decreases. A range of particle diams. and shell thicknesses is thus obtained, which can lead to the corresponding hollow capsules by exposure to hydrofluoric acid solution. The volume phase transition temperature of these materials can be easily tuned by replacing the NIPAM monomer by another N-alkylacrylamide derivative. However, the incorporation of comonomers such as acrylic acid (AA) and a phenylboronic acid (PBA) derivative inhibits the formation of core-shell structures. In order to get pH or glucose responsiveness, these functional groups can be incorporated in the outer shell of a core-double shell structure, with pNIPAM as intermediate shell. PH-responsive and glucose-responsive composite particles are obtained by this method with a high control of their internal structure.

IT 1141493-93-7P

RL: POF (Polymer in formulation); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(shell; preparation and properties of multiresponsive hybrid microgels and hollow capsules with layered structure)

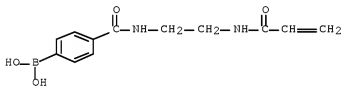
RN 1141493-93-7 ZCAPLUS

CN Boronic acid, B-[4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N,N'-methylenabis[2-propenamide] (CA INDEX NAME)

CM 1

CRN 250592-05-3

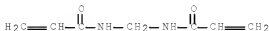
CMF C12 H15 B N2 O4



CM 2

CRN 110-26-9

CMF C7 H10 N2 O2



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 5 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2008:1229047 ZCAPLUS Full-text

DOCUMENT NUMBER: 150:24730

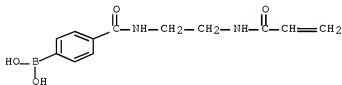
TITLE: Glucose-responsive microgels with a core-shell

structure
 AUTHOR(S): Lapeyre, Veronique; Ancla, Christophe; Catargi, Bogdan; Ravaine, Valerie
 CORPORATE SOURCE: Institut des Sciences Moleculaires, ENSCPB, Universite Bordeaux, Pessac, F-33607, Fr.
 SOURCE: Journal of Colloid and Interface Science (2008), 327(2), 316-323
 CODEN: JCISA5; ISSN: 0021-9797
 PUBLISHER: Elsevier Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB New multiresponsive core-shell microgels were synthesized, with a thermoresponsive core and a glucose-responsive shell, made resp. of poly(N-isopropylacrylamide) (pNIPAM) and pNIPAM-co-acrylamidophenylboronic acid (pNIPAM-co-APBA). The structure of the particles was elucidated by dynamic light scattering. Their thermal properties were studied and compared to those of the core alone. Without glucose, the hydrophobic shell prevented the core from swelling in a certain temperature range where the shell is collapsed. This core compression vanished upon glucose addition, when the shell became hydrophilic and swelled. Therefore, the extent of core swelling was regulated by two processes: its own internal stimulus, i.e. temperature, and shell compression, which is proportional to glucose concentration, even at physiol. salinity. The concept was applied to a selected chemical composition Core-shell microgels with a response to glucose at physiol. pH were obtained and used to encapsulate insulin. Insulin release is regulated by the presence of glucose.
 IT 701922-47-6 701922-49-8
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (shell, crosslinked; glucose-responsive microgels with core-shell structure)
 RN 701922-47-6 ZCAPLUS
 CN Boronic acid, B-[4-[[[2-[(1-oxo-2-propen-1-yl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N,N'-methylenebis[2-propenamide] and N-(1-methylethyl)-2-propenamide (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4



CM 2

CRN 2210-25-5

CMF C6 H11 N O

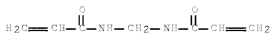
10/596571



CM 3

CRN 110-26-9

CMF C7 H10 N2 O2



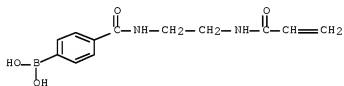
RN 701922-49-8 ZCAPLUS

CN Boronic acid, B-[4-[[[2-[(1-oxo-2-propen-1-yl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N,N'-methylenebis[2-propenamide] and 2-methyl-N-(1-methylethyl)-2-propenamide (CA INDEX NAME)

CM 1

CRN 250592-05-3

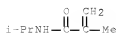
CMF C12 H15 B N2 O4



CM 2

CRN 13749-61-6

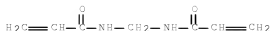
CMF C7 H13 N O



CM 3

CRN 110-26-9

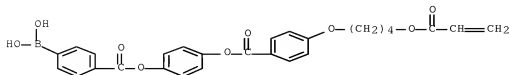
CMF C7 H10 N2 O2



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 6 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:1158940 ZCAPLUS Full-text
DOCUMENT NUMBER: 149:389773
TITLE: Optical film and polarizer
INVENTOR(S): Namikawa, Hitoshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 36pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2008225281	A	20080925	JP 2007-66087	20070315
PRIORITY APPLN. INFO.:				JP 2007-66087	20070315
AB	The invention relates to an optical film, suited for use in making a polarizer, comprising an alignment film and an optically anisotropic layer derived from a polymerizable composition containing liquid crystals, stacked in that order on a support, wherein the alignment film comprises a polymer with the average d.p. in 800-5000 and containing OH groups.				
IT	1060766-38-2				
RL	TEM (Technical or engineered material use); USES (Uses) (optically anisotropic layer; optical film and polarizer)				
RN	1060766-38-2	ZCAPLUS			
CN	Benzoic acid, 4-borono-, 1-[4-[[4-[(1-oxo-2-propen-1-yl)oxy]butoxy]benzoyl]oxy]phenyl] ester, polymer with 1,1'-(2-methyl-1,4-phenylene) bis[4-[[[4-[(1-oxo-2-propen-1-yl)oxy]butoxy]carbonyl]oxy]benzoate], α-(1-oxo-2-propen-1-yl)-ω-hydroxypoly[oxy(methyl-1,2-ethanediyl)], 2-propenoic acid and 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl 2-propenoate (CA INDEX NAME)				
CM	1				
CRN	886974-39-6				
CMF	C27 H25 B O9				



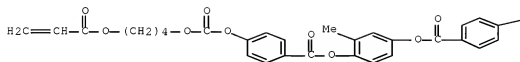
10/596571

CM 2

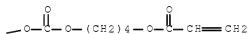
CRN 187585-64-4

CMF C37 H36 O14

PAGE 1-A



PAGE 1-B

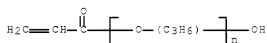


CM 3

CRN 50858-51-0

CMF (C3 H6 O)_n C3 H4 O2

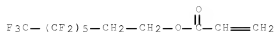
CCI IDS, PMS



CM 4

CRN 17527-29-6

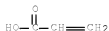
CMF C11 H7 F13 O2



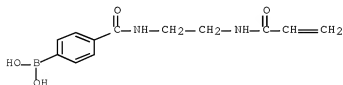
CM 5

10/596571

CRN 79-10-7
CMF C3 H4 O2



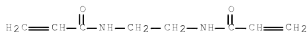
L41 ANSWER 7 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:772094 ZCAPLUS Full-text
DOCUMENT NUMBER: 149:231182
TITLE: Glucose responsive two-step release of
hydrogel-immobilized protein
AUTHOR(S): Murota, Kazutoshi; Sakamoto, Seiji; Kudo, Kazuaki
CORPORATE SOURCE: Institute of Industrial Science, The University of
Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo, 153-8505, Japan
SOURCE: Chemistry Letters (2008), 37(6), 582-583
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We designed a two-step-release system that enables protein release from
hydrogel in response to glucose. In the system, one of the heterodimeric
coiled-coil forming peptides was initially fixed to a hydrogel via a boronate-
diol interaction. The peptide was specifically released from the hydrogel by
externally incoming glucose. As a result, a protein immobilized in another
hydrogel was liberated owing to the displacement by the peptide at its
hydrogel-bound coiled-coil moiety.
IT 1043886-73-2
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(glucose responsive two-step release of hydrogel-immobilized protein)
RN 1043886-73-2 ZCAPLUS
CN Boronic acid, B-[4-[[2-[(1-oxo-2-propen-1-
yl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with
N,N'-1,2-ethanediyibis[2-propenamide] and 2-propenamide (CA INDEX NAME)
CM 1
CRN 250592-05-3
CMF C12 H15 B N2 O4



CM 2

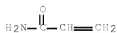
10/596571

CRN 2956-58-3
CMF C8 H12 N2 O2



CM 3

CRN 79-06-1
CMF C3 H5 N O



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 8 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:1393130 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 148:417386

TITLE: Trans-4-Iodo, 4'-boranyl-chalcone induces antitumor activity against malignant glioma cell lines in vitro and in vivo

AUTHOR(S): Sasayama, Takashi; Tanaka, Kazuhiro; Mizukawa, Katsu; Kawamura, Atsufumi; Kondoh, Takeshi; Hosoda, Kohkichi; Kohmura, Eiichi

CORPORATE SOURCE: Department of Neurosurgery, Kobe University Graduate School of Medicine, 7-5-1, Kusunoki-cho, Chuo-ku, Kobe, 650-0017, Japan

SOURCE: Journal of Neuro-Oncology (2007), 85(2), 123-132
CODEN: JNODD2; ISSN: 0167-594X

PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chalcones are considered the precursors of flavonoids and have been identified as interesting compounds with antitumor properties. Boronic-chalcone derivatives are more toxic to breast cancer cells compared to normal breast cells. Here, we studied the antitumor activities of trans-4-Iodo, 4'-boranyl-chalcone (TLBC), which is a boronic-chalcone derivative, in several glioma cell lines. TLBC showed a dose-dependent inhibition with inhibitory concentration 50% value in the μM range (5.5-25.5 μM) in various glioma cell lines. Flow cytometric and western blot assay demonstrated that TLBC induced apoptosis independent of changes to the tumor suppressor p53. This cytotoxic effect was the caspase-dependent manner. Also, TLBC lowered levels of anti-apoptotic Bcl-2 and/or Bcl-XL protein in several of the cell lines. To examine the antitumor effect of TLBC in vivo, we used a malignant glioma xenograft model. This result showed that in the mice treated with TLBC at 20 mg/kg, mean tumor volume was reduced by 43.9% ($P < 0.01$) in comparison with the control group. Immunohistochem. and western blot anal. showed that Bcl-2 protein levels were decreased and Bax protein levels were slightly increased in the tumors

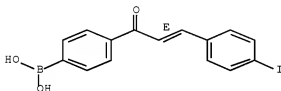
injected with 20 mg/kg TLBC compared with the control tumors. Therefore, we conclude that TLBC may be a potential chemotherapeutic agent for human glioma.

IT 562823-84-1
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (trans-4-Iodo,4'-boranyl-chalcone induced cell cycle arrest, apoptosis and decreased antiapoptotic Bcl-2 as well as Bcl-XL protein expression in human glioblastoma cell)

RN 562823-84-1 ZCAPLUS

CN Boronic acid, B-[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 9 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:90998 ZCAPLUS Full-text

DOCUMENT NUMBER: 146:158818

TITLE: Quaternary nitrogen heterocyclic compounds for detecting aqueous monosaccharides in physiological fluids

INVENTOR(S): Geddes, Chris D.; Badugu, Ramachandram; Lakowicz, Joseph R.

PATENT ASSIGNEE(S): University of Maryland Biotechnology Institute, USA

SOURCE: U.S. Pat. Appl. Publ., 72 pp., Cont.-in-part of Appl. No. PCT/US2004/022717.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070020182	A1	20070125	US 2005-318663	20051227
WO 2005000109	A2	20050106	WO 2004-US22717	20040628
WO 2005000109	A3	20050310		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,

EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-483124P P 20030627
 US 2003-483202P P 20030627
 WO 2004-US22717 A2 20040628

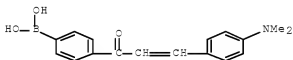
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB Quaternary nitrogen heterocyclic boronic acid-containing compds. are described, which are sensitive to glucose and fructose, as well as a variety of other physiol. important analytes, such as aqueous chloride and iodide, and a method of using the compds. Also disclosed is a contact lens doped with the quaternary nitrogen heterocyclic boronic acid-containing compound, and a method of using the doped contact lens to measure the concentration of analyte in tears under physiol. conditions.

IT 406719-92-4 406719-94-6
 RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
 (quaternary nitrogen heterocyclic compds. for detecting aqueous monosaccharides in physiol. fluids)

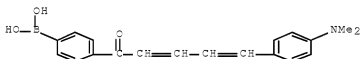
RN 406719-92-4 ZCAPLUS

CN Boronic acid, B-[4-[3-[4-(dimethylamino)phenyl]-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)



RN 406719-94-6 ZCAPLUS

CN Boronic acid, B-[4-[5-[4-(dimethylamino)phenyl]-1-oxo-2,4-pentadien-1-yl]phenyl]- (CA INDEX NAME)



L41 ANSWER 10 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2006:1179756 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:497819

TITLE: Phase difference plate with good adhesion, polymerizable compositions for it, its manufacture, and elliptic polarizer and liquid crystal display having it with wide view angle

INVENTOR(S): Yoshikawa, Susumu; Tamura, Akio

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 55pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

10/596571

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006309120	A	20061109	JP 2005-273953	20050921
KR 2006051841	A	20060519	KR 2005-91219	20050929
PRIORITY APPLN. INFO.:				
			JP 2004-285999	A 20040930
			JP 2005-93975	A 20050329

AB The phase difference plate comprises a transparent substrate, an alignment layer comprising polymer compns., and an optical anisotropy layer containing ≥ 1 liquid crystal in this order, wherein the alignment layer and/or the optical anisotropy layer contain a compound $ZnXQ$ [Z = substituent having polymerizable group; $n = 0-4$; $X = (n + 1)$ -valent linking group when $n = 1-4$; $X = H$, alkyl, alkenyl, alkynyl, aryl, heteroaryl when $n = 0$; Q = group capable of bonding to the alignment layer via adsorption] or its derivs.

IT 914100-87-1F
 RL: DEV (Device component use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
 (liquid crystal polymer phase difference plate with good adhesion for LCD with wide view angle)

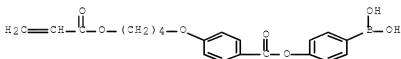
RN 914100-87-1 ZCAPLUS

CN Benzoic acid, 4-[4-[(1-oxo-2-propenyl)oxy]butoxy]-, 2,3,6,7,10,11-triphenylenehexyl ester, polymer with 4-boronophenyl 4-[4-[(1-oxo-2-propenyl)oxy]butoxy]benzoate and α -hydro- ω -[(1-oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl) ether with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (3:1) (9CI) (CA INDEX NAME)

CM 1

CRN 914100-86-0

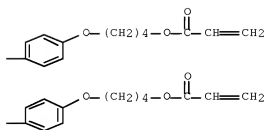
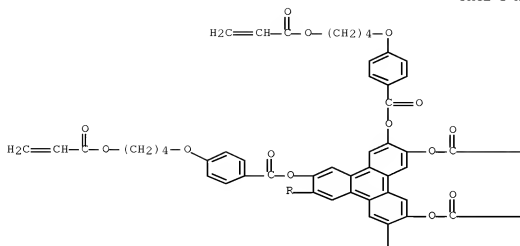
CMF C20 H21 B 07

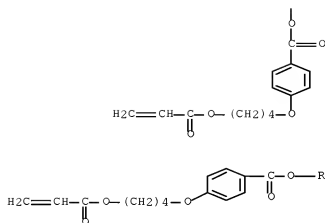


CM 2

CRN 174079-42-6

CMF C102 H96 O30



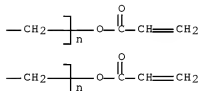
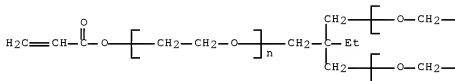


CM 3

CRN 28961-43-5

CMF (C2 H4 O)n (C2 H4 O)n (C2 H4 O)n C15 H20 O6

CCI PMS



L41 ANSWER 11 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2006:819038 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:221502

TITLE: Optical retarder films with boronic acid compound-containing anisotropic layers and liquid crystal displays therewith

INVENTOR(S): Yoshikawa, Susumu; Tamura, Akio; Ichihashi, Mitsuyoshi

10/596571

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 72pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006215093	A	20060817	JP 2005-25189	20050201
PRIORITY APPLN. INFO.:			JP 2005-25189	20050201
OTHER SOURCE(S):	MARPAT 145:221502			

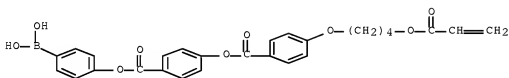
AB The retarder films comprise polymeric alignment layers and optically anisotropic layers containing (vertically oriented) rod-like liquid crystals and boronic acid compds. such as R3B(OR1)(OR2) (R1, R2 = H, aliphatic hydrocarbyl, aryl, heterocyclic group; R3 = aliphatic hydrocarbyl, aryl, heterocyclic group). Also claimed are IPS (in-plane switching)-mode liquid crystal displays having polarizer films, the above retarder films showing uniform in-plane refractive index and retardation in the thickness direction (Rth) -80 to -400 nm, and other retarder films with in-plane retardation (Re) 20-150 nm and Nz 1.5-7.

IT 904328-29-6
 RL: DEV (Device component use); MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
 (vertical orientation accelerators, retarder films; optical retarder films equipped with anisotropic layers containing vertically oriented

liquid crystals and boronates for IPC-mode LCD)

RN 904328-29-6 ZCAPLUS

CN Benzoic acid, 4-[4-[(1-oxo-2-propenyl)oxy]butoxy]-, 4-[(4-boronophenoxy)carbonyl]phenyl ester (9CI) (CA INDEX NAME)



L41 ANSWER 12 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2006:658516 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 145:262670

TITLE: A boronic-chalcone derivative exhibits potent anticancer activity through inhibition of the proteasome

AUTHOR(S): Achanta, Geetha; Modzelewska, Aneta; Feng, Li; Khan, Saeed R.; Huang, Peng

CORPORATE SOURCE: Department of Molecular Pathology, University of Texas MD Anderson Cancer Center, Houston, TX, USA

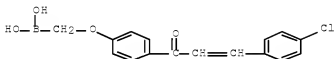
SOURCE: Molecular Pharmacology (2006), 70(1), 426-433
 CODEN: MOPMA3; ISSN: 0026-895X

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

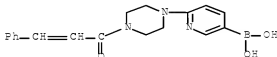
DOCUMENT TYPE: Journal

LANGUAGE: English

- AB Chalcones and their derivs. have been shown to have potent anticancer activity. However, the exact mechanisms of cytotoxic activity remain to be established. In this study, we have evaluated a series of boronic chalcones for their anticancer activity and mechanisms of action. Among the eight chalcone derivs. tested, 3,5-bis-(4-boronic acid-benzylidene)-1-methyl-piperidin-4-one (AM114) exhibited most potent growth inhibitory activity with IC50 values of 1.5 and 0.6 μ M in 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide assay and colony formation assay, resp. The cytotoxic activity of AM114 was shown to be associated with the accumulation of p53 and p21 proteins and induction of apoptosis. Mechanistic studies showed that AM114 treatment inhibited the chymotrypsin-like activity of the 20S proteasome in vitro, leading to a significant accumulation of ubiquitinated p53 and other cellular proteins in whole cells. In vitro studies showed that AM114 did not significantly disrupt the interaction of p53 and murine double minute 2 protein. It is noteworthy that AM114 as a single agent was preferentially toxic to cells with wild-type p53 expression, whereas combination of this compound with ionizing radiation (IR) significantly enhanced the cell-killing activity of IR in both wild-type p53 and p53-null cells. Together, these results indicate that the boronic chalcone derivative AM114 induces significant cytotoxic effect in cancer cells through the inhibition of the cellular proteasome and provide a rationale for the further development of this class of compds. as novel cancer chemotherapeutic agents.
- IT 888203-68-7 906533-53-7
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (boronic-chalcone derivative exhibits potent anticancer activity through inhibition of proteasome)
- RN 888203-68-7 ZCAPLUS
- CN Boronic acid, B-[[4-[3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]phenoxy]methyl]- (CA INDEX NAME)



- RN 906533-53-7 ZCAPLUS
- CN Boronic acid, B-[6-[4-(1-oxo-3-phenyl-2-propen-1-yl)-1-piperazinyl]-3-pyridinyl]- (CA INDEX NAME)



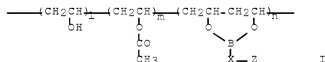
- OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
- REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/596571

ACCESSION NUMBER: 2006:464670 ZCAPLUS Full-text
 DOCUMENT NUMBER: 144:498343
 TITLE: Boric acid derivative-modified polymer films as liquid-crystal-alignment films, phase plates comprising same, and in-plane-switching liquid crystal displays
 INVENTOR(S): Tamura, Akio; Yoshikawa, Susumu
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 99 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006124639	A	20060518	JP 2005-101576	20050331
PRIORITY APPLN. INFO.:			JP 2004-285998	A 20040930

GI



AB Claimed are films made of polymers modified with boric acid derivs. ZXB(OR1)(OR2) [R1-2 = H, (substituted) aliphatic hydrocarbyl, (hetero)aryl; X = divalent connecting group, (substituted) aliphatic hydrocarbyl(ene), aryl(ene), heterocycle; Z = substituent bearing polymerizable groups; Z may be omitted]. The polymers may be poly(vinyl alc.). Also claimed are polymer films expressed by I (l + m + n = 100 mol%, l = 10-99.9, m = 0-70, n = 0.01-80). The polymer film show high adhesion to the upper- and lower films, and can speedily align liquid crystals without causing schlieren defects.

IT 886974-40-9 886974-43-2
 RL: TEM (Technical or engineered material use); USES (Uses)
 (liquid-crystal-alignment film; boric acid derivative-modified polymer film as liquid-crystal-alignment film, for phase plate and LCD)

RN 886974-40-9 ZCAPLUS

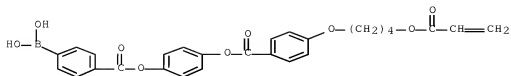
CN Benzoic acid, 4-borono-, 1-[4-[[4-[4-[(1-oxo-2-propenyl)oxy]butoxy]benzoyl]oxy]phenyl] ester, polymer with ethenol and ethenyl acetate (9CI) (CA INDEX NAME)

CM 1

CRN 886974-39-6

CMF C27 H25 B O9

10/596571



CM 2

CRN 557-75-5

CMF C2 H4 O



CM 3

CRN 108-05-4

CMF C4 H6 O2



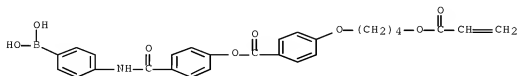
RN 886974-43-2 ZCAPLUS

CN Benzoic acid, 4-[4-[(1-oxo-2-propenyl)oxy]butoxy]-, 4-[[4-(4-boronophenyl)amino]carbonyl]phenyl ester, polymer with ethenol and ethenyl acetate (9CI) (CA INDEX NAME)

CM 1

CRN 886974-42-1

CMF C27 H26 B N O8



CM 2

CRN 557-75-5

CMF C2 H4 O

10/596571



CM 3

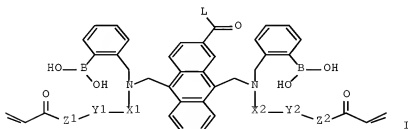
CRN 108-05-4
CMF C4 H6 O2



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L41 ANSWER 14 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:363151 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 144:419779
TITLE: Fluorescent monomer compounds and blood sugar
level-detecting sensing substances and their use in
body implant
INVENTOR(S): Kawanishi, Tetsuo; Ochiai, Shoji
PATENT ASSIGNEE(S): Terumo Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006104140	A	20060420	JP 2004-294413	20041007
PRIORITY APPLN. INFO.: GI			JP 2004-294413	20041007



AB The title substances particularly useful for diabetic patients, are obtained from the copolymers of (meth)acrylamide monomers and comonomers bearing sugar-

bondable hydrophobic groups which become fluorescent after bonding with sugar and have hydrophilic groups. Suitable comonomers are compds. having structure of I (X1,X2 = COO, OCO, CH2NR, Natural Rubber, NRCO, CONR, SO2NR, NRSO2, O, S, SS, NRCOO, OCONR, CO, C1-30 alkylene; R = H, alkyl; Z1,Z2 = O, NR'; R' = H, alkyl; Y1,Y2 = linking groups; L = C1-10 alkyl groups).

IT 883724-03-6P

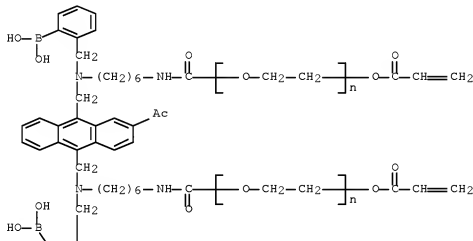
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(manufacture of fluorescent copolymers for implantable blood sugar level-detecting sensors)

RN 883724-03-6 ZCAPLUS

CN Poly(oxy-1,2-ethanediyl), α,α' -[(2-acetyl-9,10-anthracenediyl)bis[methylene[[(2-boronophenyl)methyl]imino]-6,1-hexanediyliminocarbonyl]]bis[ω -[(1-oxo-2-propenyl)oxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



IT 883724-04-7P

RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(manufacture of fluorescent copolymers for implantable blood sugar level-detecting sensors)

RN 883724-04-7 ZCAPLUS

CN 2-Propenamide, N,N'-methylenebis-, polymer with α,α' -[(2-acetyl-9,10-anthracenediyl)bis[methylene[[(2-boronophenyl)methyl]imino]-6,1-hexanediyliminocarbonyl]]bis[ω -[(1-

10/596571

oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl)] and 2-propenamide (9CI) (CA INDEX NAME)

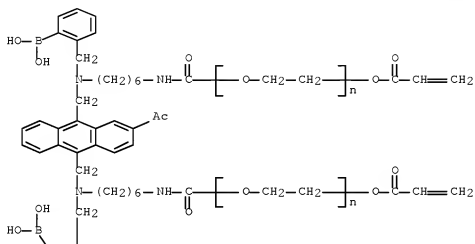
CM 1

CRN 883724-03-6

CMF (C2 H4 O)n (C2 H4 O)n C52 H62 B2 N4 O11

CCI PMS

PAGE 1-A



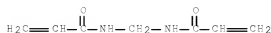
PAGE 2-A



CM 2

CRN 110-26-9

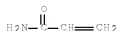
CMF C7 H10 N2 O2



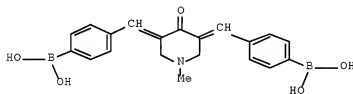
CM 3

10/596571

CRN 79-06-1
CMF C3 H5 N O



L41 ANSWER 15 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:315088 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:290
TITLE: Anticancer activities of novel chalcone and
bis-chalcone derivatives
AUTHOR(S): Modzelewska, Aneta; Pettit, Catherine; Achanta,
Geetha; Davidson, Nancy E.; Huang, Peng; Khan, Saeed
R.
CORPORATE SOURCE: Division of Chemical Therapeutics, Sidney Kimmel
Comprehensive Cancer Center at Johns Hopkins,
Baltimore, MD, 21231, USA
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(10),
3491-3495
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:290
GI



I

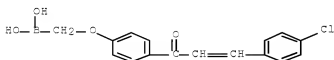
- AB A series of novel chalcones and bis-chalcones containing boronic acid moieties has been synthesized and evaluated for antitumor activity against the human breast cancer MDA-MB-231 (estrogen receptor-neg.) and MCF7 (estrogen receptor-pos.) cell lines and against two normal breast epithelial cell lines, MCF-10A and MCF-12A. These mols. inhibited the growth of the human breast cancer cell lines at low micromolar to nanomolar concns., with five of them showing preferential inhibition of the human breast cancer cell lines. Furthermore, bis-chalcone I exhibited a more potent inhibition of colon cancer cells expressing wild-type p53 than of an isogenic cell line that was p53-null.
- IT 888203-68-7P 888203-69-8P 888203-70-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/596571

(anticancer activities of chalcone and bis-chalcone derivs.)

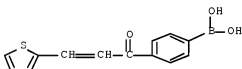
RN 888203-68-7 ZCAPLUS

CN Boronic acid, B-[[4-[3-(4-chlorophenyl)-1-oxo-2-propen-1-yl]phenoxy]methyl]- (CA INDEX NAME)



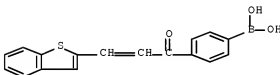
RN 888203-69-8 ZCAPLUS

CN Boronic acid, B-[4-[1-oxo-3-(2-thienyl)-2-propen-1-yl]phenyl]- (CA INDEX NAME)



RN 888203-70-1 ZCAPLUS

CN Boronic acid, B-[4-(3-benzo[b]thien-2-yl-1-oxo-2-propen-1-yl)phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (26 CITINGS)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 16 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2006:69817 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 144:159854

TITLE: Glucose-measuring fluorescent monomer, glucose-measuring fluorescent sensor polymer substance, and implantable glucose-measuring sensor

INVENTOR(S): Ochiai, Shouji; Kawanishi, Tetsuro; Matsumoto, Atsushi

PATENT ASSIGNEE(S): Terumo Kabushiki Kaisha, Japan

SOURCE: Eur. Pat. Appl., 41 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

10/596571

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1619229	A1	20060125	EP 2005-15807	20050720
EP 1619229	B1	20070411		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
JP 2006036664	A	20060209	JP 2004-216535	20040723
JP 2006111719	A	20060427	JP 2004-299991	20041014
AT 359339	T	20070515	AT 2005-15807	20050720
CN 1900212	A	20070124	CN 2005-10085192	20050722
US 20060020182	A1	20060126	US 2005-187821	20050725
US 7388110	B2	20080617		
US 20080021236	A1	20080124	US 2007-890518	20070807
US 7524985	B2	20090428		
US 20080319288	A1	20081225	US 2008-222579	20080812
PRIORITY APPLN. INFO.:			JP 2004-216535	A 20040723
			JP 2004-299991	A 20041014
			US 2005-187821	A3 20050725
			US 2007-890518	A3 20070807
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT				
OTHER SOURCE(S): CASREACT 144:159854; MARPAT 144:159854				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The fluorescent monomer compds. are represented by formula (I), where Q, Q' and D3 may be the same or different, may be combined together into a fused ring, and are, for example, H, a halogen atom, OH, or a substituted or unsubstituted alkyl group; and D1, D2 and D4 each represent a substituent with a vinyl group at the end. The fluorescent monomer compds. are soluble in water. Me 9,10-dimethylantracene-2-carboxylate was successively brominated at 9,10-methyls, methylaminated, and reacted with 2-(bromomethyl)benzeneboronic acid protected as a dioxaborinane. After hydrolysis, thus obtained anthracene-2-carboxylic acid (70 mg) was amidated by 1-acrylamido-6-aminoheptane to give the target fluorescent monomer 9,10-bis([N-methyl-N-(ortho-boronobenzyl)amino]methyl)anthracene (85 mg). The fluorescent sensor substance was prepared either by (1) direct copolymn. of the fluorescent monomer with acrylamide at different ratios (producing copolymers containing fluorescent monomer:acrylamide molar ratios from 1:10 to 1:3874), or by (2) amidation of the above intermediate anthracene-2-carboxylic acid with amino- and acrylamido-terminated PEG3400 followed by copolymn. with acrylamide. The prepared polymers were used in phosphate buffer (pH 7) solns. as glucose-measuring fluorescent sensors. The polymer concentration was adjusted so that absorbance at 265 nm would become 0.05; the glucose concentration was 500 mg/dL. The best result was obtained in method (2) with relative fluorescence intensity I/I₀ about 7 (excitation 405 nm, emission 442 nm). The copolymer of synthesized compound (II) with acrylamide and N,N'-methylenebis(acrylamide) was immobilized on a glass support, and the detector layer was prepared. The detector layer was held in place on the evaluation device, and the fluorescence response to glucose at varied concns. under phosphate buffer (pH 7) was measured (I/I₀ = 10, excitation 400 nm, emission 480 nm, glucose concentration 500 mg/dL).

IT 873555-16-9P

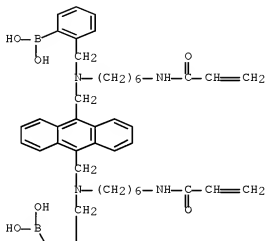
10/596571

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(comparative example; copolymn.; glucose-measuring fluorescent monomer, glucose-measuring fluorescent sensor polymer substance, and implantable glucose-measuring sensor)

RN 873555-16-9 ZCAPLUS

CN Boronic acid, [9,10-anthracenediylbis[methylene[[6-[(1-oxo-2-propenyl)amino]hexyl]imino]methylene-2,1-phenylene]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



IT 873555-19-2P 873555-24-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(copolymn.; glucose-measuring fluorescent monomer, glucose-measuring fluorescent sensor polymer substance, and implantable glucose-measuring sensor)

RN 873555-19-2 ZCAPLUS

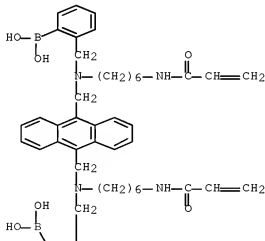
CN Poly(oxy-1,2-ethanediyl), α, α' -[(2-acetyl-9,10-anthracenediyl)bis[methylene[[(2-boronophenyl)methyl]imino]-6,1-hexanediylimino(2-oxo-2,1-ethanediyl)]]bis[ω -[(1-oxo-2-propenyl)oxy]-(9CI) (CA INDEX NAME)

PAGE 2-A



IT 873555-17-0P 873555-26-1P
 RL: ARG (Analytical reagent use); DEV (Device component use); DGN (Diagnostic use); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (glass-supported; comparative example; glucose-measuring fluorescent monomer, glucose-measuring fluorescent sensor polymer substance, and implantable glucose-measuring sensor)
 RN 873555-17-0 ZCAPLUS
 CN Boronic acid, [9,10-anthracenediylbis[methylene[[6-[(1-oxo-2-propenyl)amino]hexyl]imino]methylene-2,1-phenylene]]bis-, polymer with 2-propenamide (9CI) (CA INDEX NAME)
 CM 1
 CRN 873555-16-9
 CMF C48 H60 B2 N4 O6

PAGE 1-A

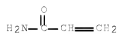




CM 2

CRN 79-06-1

CMF C3 H5 N O



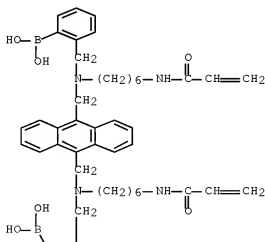
RN 873555-26-1 ZCAPLUS

CN Boronic acid, [9,10-anthracenediylbis[methylene[6-[(1-oxo-2-propenyl)amino]hexyl]imino)methylene-2,1-phenylene]]bis-, polymer with N,N'-methylenebis[2-propenamide] and 2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 873555-16-9

CMF C48 H60 B2 N4 O6

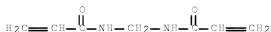




CM 2

CRN 110-26-9

CMF C7 H10 N2 O2



CM 3

CRN 79-06-1

CMF C3 H5 N O



IT 873555-20-5P 873555-25-0P

RL: ARG (Analytical reagent use); DEV (Device component use); DGN (Diagnostic use); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (glass-supported; glucose-measuring fluorescent monomer, glucose-measuring fluorescent sensor polymer substance, and implantable glucose-measuring sensor)

RN 873555-20-5 ZCAPLUS

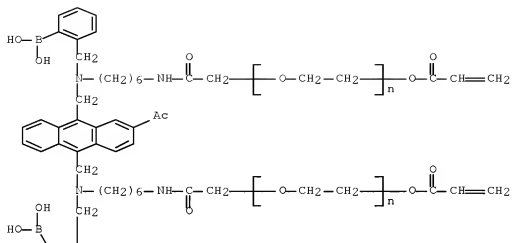
CN 2-Propenamide, N,N'-methylenebis-, polymer with
 α,α' -[(2-acetyl-9,10-anthracenediyl)bis[methylene[[(2-boronophenyl)methyl]imino]-6,1-hexanediylimino(2-oxo-2,1-ethanediyl)]]bis[θ -[(1-oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl)] and 2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 873555-19-2

CMF (C2 H4 O)_n (C2 H4 O)_n C54 H66 B2 N4 O11

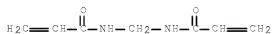
CCI PMS



CM 2

CRN 110-26-9

CMF C7 H10 N2 O2



CM 3

CRN 79-06-1

CMF C3 H5 N O



10/596571

RN 873555-25-0 ZCAPLUS

CN 2-Propenamide, N,N'-methylenebis-, polymer with
 α, α' -[2-(methoxycarbonyl)-9,10-anthracenediyl]bis[methylene[[(2-boronophenyl)methyl]imino]-6,1-hexanediylimino(2-oxo-2,1-ethanediyl)]bis[6-[(1-oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl)] and 2-propenamide (9CI) (CA INDEX NAME)

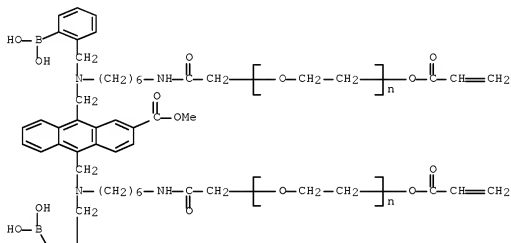
CM 1

CRN 873555-24-9

CMF (C2 H4 O)_n (C2 H4 O)_n C54 H66 B2 N4 O12

CCI PMS

PAGE 1-A



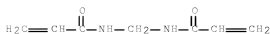
PAGE 2-A



CM 2

CRN 110-26-9

CMF C7 H10 N2 O2



CM 3

CRN 79-06-1

CMF C3 H5 N O



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 17 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:1114291 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:58663

TITLE: A glucose-sensing contact lens: a new approach to
noninvasive continuous physiological glucose
monitoringAUTHOR(S): Badugu, Ramachandram; Lakowicz, Joseph R.; Geddes,
Chris D.CORPORATE SOURCE: Cent. fluorescence Spectroscopy, Dep. Biochem. & Mol.
Biol., Univ. of Maryland School of Medicine, MD,
21201, USASOURCE: Proceedings of SPIE-The International Society for
Optical Engineering (2004), 5317(Optical Fibers and
Sensors for Medical Applications IV), 234-245
CODEN: PSISDG; ISSN: 0277-786X

PUBLISHER: SPIE-The International Society for Optical Engineering

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors have developed a new technol. for the non-invasive continuous
monitoring of tear glucose using a daily use, disposable contact lens,
embedded with sugar-sensing boronic acid containing fluorophores. The
authors' findings show that the authors' approach may be suitable for the
continuous monitoring of tear glucose levels in the range 50-500 μM , which
track blood glucose levels that are typically \approx 5-10-fold higher. The authors
initially tested the sensing concept with well-established, previously
published, boronic acid probes and the results could conclude the used probes,
with higher pKa values, are almost insensitive toward glucose within the
contact lens, attributed to the low pH and polarity inside the lens.
Subsequently, the authors have developed a range of probes based on the
quinolinium backbone, having considerably lower pKa values, which enables them
to be suitable to sense the physiol. glucose in the acidic pH contact lens.
Herein the authors describe the results based on the authors' findings towards
the development of glucose sensing contact lens and therefore an approach to
non-invasive continuous monitoring of tear glucose using a contact lens.

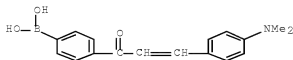
IT 406719-92-4, Chalc 1

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
(Uses)

(noninvasive continuous physiol. glucose monitoring in contact lens)

RN 406719-92-4 ZCAPLUS

CN Boronic acid, B-[4-[3-[4-(dimethylamino)phenyl]-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 18 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:952799 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:398794

TITLE: Monitoring the Effects of Antagonists on Protein-Protein Interactions with NMR Spectroscopy

AUTHOR(S): D'Silva, Loyola; Ozdowy, Przemyslaw; Krajewski, Marcin; Rothweiler, Ulli; Singh, Mahavir; Holak, Tad A.

CORPORATE SOURCE: Max Planck Institute for Biochemistry, Martinsried, D-82152, Germany

SOURCE: Journal of the American Chemical Society (2005), 127(38), 13220-13226

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe an NMR method that directly monitors the influence of ligands on protein-protein interactions. For a two-protein interaction complex, the size of one component should be small enough (less than .apprx.15 kDa) to provide a good quality 15N (13C) HSQC spectrum after 15N(13C) labeling. The size of the second unlabeled component should be large enough so that the mol. weight of the preformed complex is larger than .apprx. 40 kDa. When the smaller protein binds to a larger one, broadening of NMR resonances results in the disappearance of most of its cross-peaks in the HSQC spectrum. Addition of an antagonist that can dissociate the complex would restore the HSQC spectrum of the smaller component. The method directly shows whether an antagonist releases proteins in their wild-type folded states or whether it induces their denaturation, partial unfolding, or precipitation. We illustrate the method by studying lead compds. that have recently been reported to block the MDM2-p53 interaction. Activation of p53 in tumor cells by inhibiting its interaction with MDM2 offers new strategy for cancer therapy.

IT 562823-90-9

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

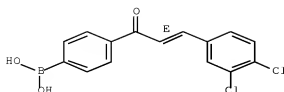
(Biological study); USES (Uses)

(monitoring effects of antagonists on protein-protein interactions with NMR spectroscopy)

RN 562823-90-9 ZCAPLUS

CN Boronic acid, [4-[1(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)
 REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 19 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:141046 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 142:219141

TITLE: Preparation of benzofuran derivatives useful for treating hyperproliferative disorders

INVENTOR(S): Zhang, Chengzhi; Dumas, Jacques; Ladouceur, Gaetan H.; Zhao, Qian; Hentemann, Martin F.; Verma, Sharad K.; Zhu, Qingming; Lavoie, Rico C.; Fan, Jianmei; Phillips, Barton

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 128 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

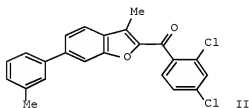
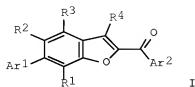
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005014566	A1	20050217	WO 2004-US25480	20040806
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2534678	A1	20050217	CA 2004-2534678	20040806
EP 1654245	A1	20060510	EP 2004-780334	20040806
R:	DE, ES, FR, GB, IT			
JP 2007501796	T	20070201	JP 2006-522757	20040806
US 20060194816	A1	20060831	US 2006-566343	20060127
US 7420066	B2	20080902		
US 20090023783	A1	20090122	US 2008-201547	20080829
US 20090292014	A1	20091126	US 2009-471335	20090522
PRIORITY APPLN. INFO.:			US 2003-494165P	P 20030807
			WO 2004-US25480	W 20040806
			US 2006-566343	A3 20060127
			US 2008-201547	A1 20080829

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

10/596571

OTHER SOURCE(S):
GI

CASREACT 142:219141; MARPAT 142:219141



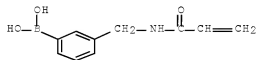
AB Title compds. I [wherein Ar1 = benzodioxolyl, pyrrolidinyl, (un)substituted pyridinyl, Ph, etc.; Ar2 = benzodioxolyl, (un)substituted Ph, pyridinyl; R1 = H, alkyl, OH, halo; R2 = H, alkyl, alkoxy, OH, halo, CF3, OCF3; R3 = H, alkoxy, OH, halo, CF3; R4 = H, alkyl, alkoxy, CN, etc.; and their pharmaceutically acceptable salts] were prepared as medicaments for the treatment or prophylaxis of disorders, especially of hyperproliferative disorders. For example, II was prepared by cyclocondensation of 1-(4-bromo-2-hydroxyphenyl)ethanone (preparation given) with 2-chloro-1-(2,4-dichlorophenyl)ethanone, and Pd-cross coupling of bromide with 3-methylphenylboronic acid. Selected I inhibited H460 lung carcinoma cells proliferation (IC50 < 10 μ M) in an in vitro assay. Thus, I are useful as antiproliferative agents for treating neoplasm.

IT 939992-88-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzofurans as antiproliferative agents)

RN 939992-88-8 ZCAPLUS

CN Boronic acid, B-[3-[(1-oxo-2-propen-1-yl)amino]methyl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 20 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2005:14124 ZCAPLUS Full-text
 DOCUMENT NUMBER: 142:89411
 TITLE: Quaternary nitrogen heterocyclic compounds for
 detecting aqueous monosaccharides in physiological
 fluids
 INVENTOR(S): Geddes, Chris D.; Badugu, Ramachandran; Lakowitz,
 Joseph R.
 PATENT ASSIGNEE(S): University of Maryland Biotechnology Institute, USA
 SOURCE: PCT Int. Appl., 120 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005000109	A2	20050106	WO 2004-US22717	20040628
WO 2005000109	A3	20050310		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1644330	A2	20060412	EP 2004-778295	20040628
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK			
US 20070020182	A1	20070125	US 2005-318663	20051227
PRIORITY APPLN. INFO.:			US 2003-483124P	P 20030627
			US 2003-483202P	P 20030627
			WO 2004-US22717	W 20040628

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 142:89411

AB Disclosed are quaternary nitrogen heterocyclic boronic acid-containing compds. which are sensitive to glucose and fructose, as well as a variety of other physiol. important analytes, such as aqueous chloride and iodide, and a method of using the compds. Also disclosed is a contact lens doped with the quaternary nitrogen heterocyclic boronic acid-containing compound, and a method of using the doped contact lens to measure the concentration of analyte in tears under physiol. conditions.

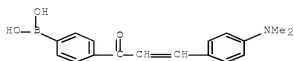
IT 406719-92-4 406719-94-6

RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)

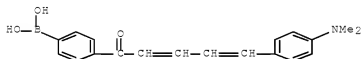
(quaternary nitrogen heterocyclic compds. for detecting aqueous monosaccharides in physiol. fluids)

RN 406719-92-4 ZCAPLUS

CN Boronic acid, B-[4-[3-[4-(dimethylamino)phenyl]-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)



RN 406719-94-6 ZCAPLUS
 CN Boronic acid, B-[4-[5-[4-(dimethylamino)phenyl]-1-oxo-2,4-pentadien-1-yl]phenyl]- (CA INDEX NAME)



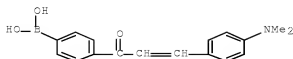
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
 REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 21 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2004:621102 ZCAPLUS Full-text
 DOCUMENT NUMBER: 142:234524
 TITLE: Cyanide-sensitive fluorescent probes
 AUTHOR(S): Badugu, Ramachandram; Lakowicz, Joseph R.; Geddes, Chris D.
 CORPORATE SOURCE: Center for Fluorescence Spectroscopy, Department of Biochemistry and Molecular Biology, Medical Biotechnology Center, University of Maryland School of Medicine, Baltimore, MD, 21201, USA
 SOURCE: Dyes and Pigments (2005), 64(1), 49-55
 CODEN: DYPIDX; ISSN: 0143-7208
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB We characterize the response of several boronic acid containing fluorophores, which are widely used for sugar determination, towards aqueous cyanide. In two recent reports we have shown that boronic acid containing fluorophores can be used to sense aqueous cyanide through physiol. safeguard levels. In this report we show that our new sensing mechanism is not just specific to our recently reported probes, but is indeed generic to the boronic acid moiety itself. Subsequently a wide range of cyanide-sensitive probes can now be realized, offering several modalities for fluorescence based cyanide sensing such as: intensity, lifetime, ratiometric, polarization and modulation fluorescence sensing.

IT 406719-92-4, Chalc 1
 RL: ARG (Analytical reagent use); PRP (Properties); ANST (Analytical study); USES (Uses)
 (cyanide sensing by boronic acid-containing fluorescent probes)

RN 406719-92-4 ZCAPLUS
 CN Boronic acid, B-[4-[3-[4-(dimethylamino)phenyl]-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 35 THERE ARE 35 CAPLUS RECORDS THAT CITE THIS RECORD (35 CITINGS)
 REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 22 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2004:453269 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 141:24150
 TITLE: Polymeric boronic acid derivatives as lipase inhibitors, (macro)monomer precursors, and treatment of obesity
 INVENTOR(S): Huval, Chad Cori; Li, Xinhua; Holmes-Farley, Stephen Randall; Dhal, Pradeep K.
 PATENT ASSIGNEE(S): Genzyme Corporation, USA
 SOURCE: PCT Int. Appl., 94 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046211	A1	20040603	WO 2003-US36861	20031119
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2546696	A1	20040603	CA 2003-2546696	20031119
AU 2003291567	A1	20040615	AU 2003-291567	20031119
EP 1578816	A1	20050928	EP 2003-768974	20031119
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
US 20060134062	A1	20060622	US 2005-535639	20051221
PRIORITY APPLN. INFO.:			US 2002-427518P	P 20021119
			WO 2003-US36861	W 20031119

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB Human obesity is a health problem affecting a significant proportion of the American population. Numerous methods of treating obesity and reducing absorption of fat were developed, but all have serious drawbacks. A novel class of polymers with either a S atom or an electron withdrawing group between a polymer backbone and pendant aryl boronic acid group is prepared. Polymers having such an electron withdrawing group are particularly effective in inhibiting lipase in vitro and in vivo. Thus, 1.0 g 4-(13'-acryloxy-2'-thia)tridecylphenylboronic acid (preparation given), 20 mg AIBN, and 5 mL EtOH

10/596571

was stirred, the reaction mixture was heated to 65° and stirred 24 h under N atmospheric, after the addition of 10 mg AIBN, heating continued for addnl. 24 h to give crude polymer.

IT 698361-07-8P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(polymeric boronic acid-pendant derivs. as lipase inhibitors for treatment of obesity)

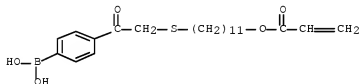
RN 698361-07-8 ZCAPLUS

CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester, polymer with 1-(1-oxo-2-propenyl)-2,5-pyrrolidinedione (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

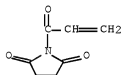
CMF C22 H33 B O5 S



CM 2

CRN 56905-55-6

CMF C7 H7 N O3



IT	698360-11-1P	698360-13-3P	698360-15-5P
	698360-17-7P	698360-19-9P	698360-21-3P
	698360-22-4P	698360-24-6P	698360-26-8P
	698360-29-1P	698360-31-5P	698360-33-7P
	698360-35-9P	698360-37-1P	698360-40-6P
	698360-42-8P	698360-45-1P	698360-48-4P
	698360-50-9P	698360-59-7P	698360-62-2P
	698360-65-5P	698360-67-7P	698360-78-0P
	698360-80-4P	698360-83-7P	698360-86-0P
	698360-89-3P	698360-92-8P	698360-95-1P
	698360-98-4P	698361-01-2P	698361-03-4P
	698361-05-6P	698361-10-3P	698382-85-3P

RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/596571

(polymeric boronic acid-pendant derivs. as lipase inhibitors for treatment of obesity)

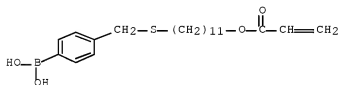
RN 698360-11-1 ZCAPLUS

CN 2-Propenoic acid, 11-[[[4-(boronophenyl)methyl]thio]undecyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 698358-73-5

CMF C21 H33 B O4 S



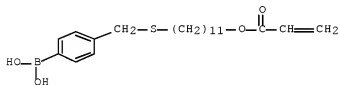
RN 698360-13-3 ZCAPLUS

CN 2-Propenoic acid, 11-[[[4-(boronophenyl)methyl]thio]undecyl ester, polymer with 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid monosodium salt (9CI) (CA INDEX NAME)

CM 1

CRN 698358-73-5

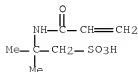
CMF C21 H33 B O4 S



CM 2

CRN 5165-97-9

CMF C7 H13 N O4 S . Na



● Na

10/596571

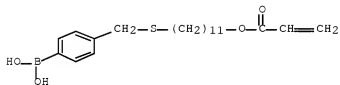
RN 698360-15-5 ZCAPLUS

CN 2-Propenoic acid, 11-[[[4-(4-boronophenyl)methyl]thio]undecyl ester, polymer with N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698358-73-5

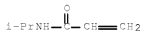
CMF C21 H33 B O4 S



CM 2

CRN 2210-25-5

CMF C6 H11 N O



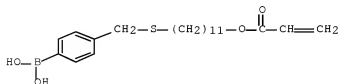
RN 698360-17-7 ZCAPLUS

CN 2-Propenoic acid, 11-[[[4-(4-boronophenyl)methyl]thio]undecyl ester, polymer with N,N-diethyl-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698358-73-5

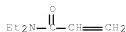
CMF C21 H33 B O4 S



CM 2

10/596571

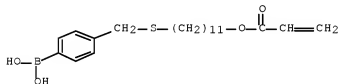
CRN 2675-94-7
CMF C7 H13 N O



RN 698360-19-9 ZCAPLUS
CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride, polymer with 11-[[4-(boronophenyl)methyl]thio]undecyl 2-propenoate and N,N-diethyl-2-propenamide (9CI) (CA INDEX NAME)

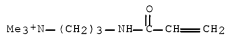
CM 1

CRN 698358-73-5
CMF C21 H33 B O4 S



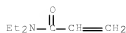
CM 2

CRN 45021-77-0
CMF C9 H19 N2 O . Cl



CM 3

CRN 2675-94-7
CMF C7 H13 N O



10/596571

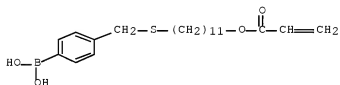
RN 698360-21-3 ZCAPLUS

CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride, polymer with 11-[[[4-boronophenyl)methyl]thio]undecyl 2-propenoate and 2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698358-73-5

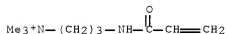
CMF C21 H33 B O4 S



CM 2

CRN 45021-77-0

CMF C9 H19 N2 O . Cl



● Cl⁻

CM 3

CRN 79-06-1

CMF C3 H5 N O



RN 698360-22-4 ZCAPLUS

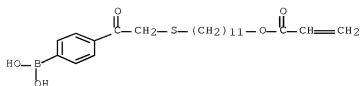
CN 2-Propenoic acid, 11-[[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

CMF C22 H33 B O5 S

10/596571



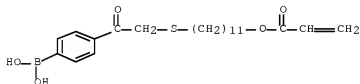
RN 698360-24-6 ZCAPLUS

CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester,
polymer with 2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

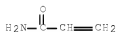
CMF C22 H33 B O5 S



CM 2

CRN 79-06-1

CMF C3 H5 N O



RN 698360-26-8 ZCAPLUS

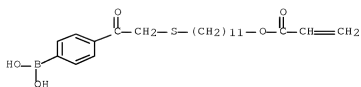
CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride,
polymer with 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl 2-propenoate
(9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

CMF C22 H33 B O5 S

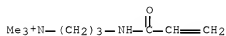
10/596571



CM 2

CRN 45021-77-0

CMF C9 H19 N2 O . Cl



● Cl⁻

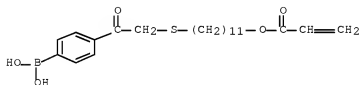
RN 698360-29-1 ZCAPLUS

CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester, polymer with 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid monosodium salt (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

CMF C22 H33 B O5 S

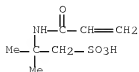


CM 2

CRN 5165-97-9

CMF C7 H13 N O4 S . Na

10/596571



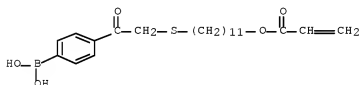
RN 698360-31-5 ZCAPLUS

CN 2-Propenoic acid, polymer with 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

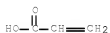
CMF C22 H33 B O5 S



CM 2

CRN 79-10-7

CMF C3 H4 O2



RN 698360-33-7 ZCAPLUS

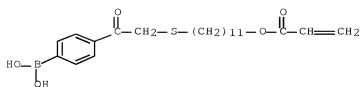
CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester, polymer with sodium 4-ethenylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

CMF C22 H33 B O5 S

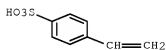
10/596571



CM 2

CRN 2695-37-6

CMF C8 H8 O3 S . Na



● Na

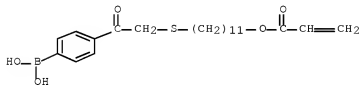
RN 698360-35-9 ZCAPLUS

CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride, polymer with 11-[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl 2-propenoate and 2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

CMF C22 H33 B O5 S

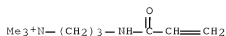


CM 2

CRN 45021-77-0

CMF C9 H19 N2 O . Cl

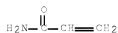
10/596571



CM 3

CRN 79-06-1

CMF C3 H5 N O



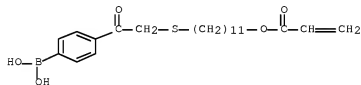
RN 698360-37-1 ZCAPLUS

CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride, polymer with 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl 2-propenoate and 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid monosodium salt (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

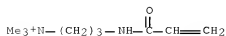
CMF C22 H33 B O5 S



CM 2

CRN 45021-77-0

CMF C9 H19 N2 O . Cl

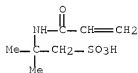


10/596571

CM 3

CRN 5165-97-9

CMF C7 H13 N O4 S . Na



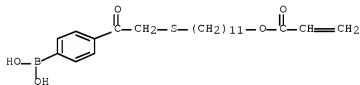
RN 698360-40-6 ZCAPLUS

CN 1-Propanaminium, N,N-dimethyl-N-[3-[(2-methyl-1-oxo-2-propenyl)amino]propyl]-3-sulfo-, inner salt, polymer with 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

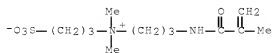
CMF C22 H33 B O5 S



CM 2

CRN 5205-95-8

CMF C12 H24 N2 O4 S



RN 698360-42-8 ZCAPLUS

CN 1-Propanaminium, N,N-dimethyl-N-[3-[(2-methyl-1-oxo-2-

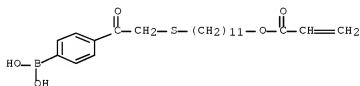
10/596571

propenyl)amino]propyl]-3-sulfo-, inner salt, polymer with
 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl 2-propenoate and
 N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-1-propanaminium chloride (9CI)
 (CA INDEX NAME)

CM 1

CRN 698358-86-0

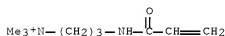
CMF C22 H33 B O5 S



CM 2

CRN 45021-77-0

CMF C9 H19 N2 O . Cl

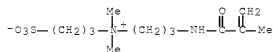


● Cl⁻

CM 3

CRN 5205-95-8

CMF C12 H24 N2 O4 S



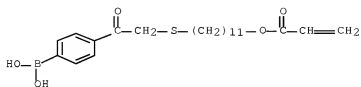
RN 698360-45-1 ZCAPLUS

CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester,
 polymer with 3-sulfopropyl 2-propenoate potassium salt (9CI) (CA INDEX
 NAME)

CM 1

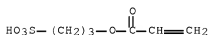
10/596571

CRN 698358-86-0
CMF C22 H33 B O5 S



CM 2

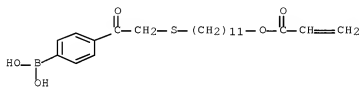
CRN 31098-20-1
CMF C6 H10 O5 S . K



RN 698360-48-4 ZCAPLUS
CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester,
polymer with [(4-ethenylphenyl)methyl]phosphonic acid (9CI) (CA INDEX
NAME)

CM 1

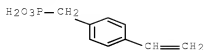
CRN 698358-86-0
CMF C22 H33 B O5 S



CM 2

CRN 53459-43-1
CMF C9 H11 O3 P

10/596571

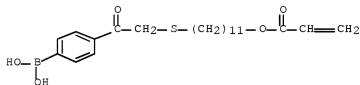


RN 698360-50-8 ZCAPLUS
 CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester,
 polymer with α -(1-oxo-2-propenyl)- ω -methoxypoly(oxy-1,2-ethanediyl), graft (9CI) (CA INDEX NAME)

CM 1

CRN 698358-86-0

CMF C22 H33 B O5 S

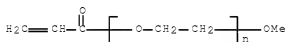


CM 2

CRN 32171-39-4

CMF (C2 H4 O)n C4 H6 O2

CCI PMS



RN 698360-59-7 ZCAPLUS
 CN 2-Propenoic acid, 6-[[2-(4-boronophenyl)-2-oxoethyl]thio]hexyl ester,
 polymer with 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid
 monosodium salt (9CI) (CA INDEX NAME)

CM 1

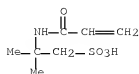
CRN 698359-23-8

CMF C17 H23 B O5 S

O=P(O)(O)c1ccc(cc1)C(=O)OCCSCCOC(=O)C=C
$$\begin{array}{c} \text{O} \\ \parallel \\ \text{NH}-\text{C}-\text{CH}=\text{CH}_2 \\ | \\ \text{Me}-\text{C}-\text{CH}_2-\text{SO}_3\text{H} \\ | \\ \text{Me} \end{array}$$
O=P(O)(O)c1ccc(cc1)C(=O)CCSCCOC(=O)C=C

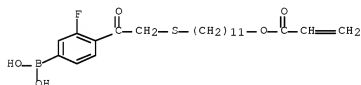
101

10/596571

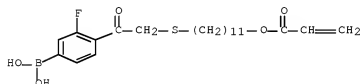


● Na

RN 698360-65-5 ZCAPLUS
 CN 2-Propenoic acid, 11-[(2-(4-borono-2-fluorophenyl)-2-oxoethyl)thio]undecyl ester, homopolymer (9CI) (CA INDEX NAME)
 CM 1
 CRN 698359-33-0
 CMF C22 H32 B F O5 S

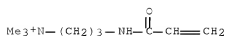


RN 698360-67-7 ZCAPLUS
 CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride, polymer with 11-[(2-(4-borono-2-fluorophenyl)-2-oxoethyl)thio]undecyl 2-propenoate (9CI) (CA INDEX NAME)
 CM 1
 CRN 698359-33-0
 CMF C22 H32 B F O5 S



CM 2
 CRN 45021-77-0
 CMF C9 H19 N2 O . Cl

10/596571



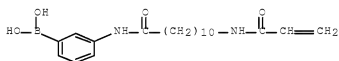
RN 698360-78-0 ZCAPLUS

CN Boronic acid, [3-[1-oxo-11-[(1-oxo-2-propenyl)amino]undecyl]amino]phenyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 698359-88-5

CMF C20 H31 B N2 O4



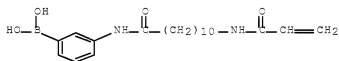
RN 698360-80-4 ZCAPLUS

CN Boronic acid, [3-[[1-oxo-11-[(1-oxo-2-propenyl)amino]undecyl]amino]phenyl]-, polymer with N,N-diethyl-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698359-88-5

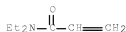
CMF C20 H31 B N2 O4



CM 2

CRN 2675-94-7

CMF C7 H13 N O



10/596571

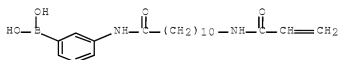
RN 698360-83-7 ZCAPLUS

CN Boronic acid, [3-[[1-oxo-11-[(1-oxo-2-propenyl)amino]undecyl]amino]phenyl]-, polymer with N-butyl-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698359-88-5

CMF C20 H31 B N2 O4



CM 2

CRN 2565-18-6

CMF C7 H13 N O



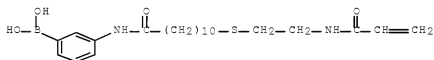
RN 698360-86-0 ZCAPLUS

CN Boronic acid, [3-[[1-oxo-11-[[2-[(1-oxo-2-propenyl)amino]ethyl]thio]undecyl]amino]phenyl]-, polymer with N-butyl-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698359-82-9

CMF C22 H35 B N2 O4 S



CM 2

CRN 2565-18-6

CMF C7 H13 N O

10/596571



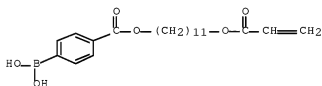
RN 698360-89-3 ZCAPLUS

CN Benzoic acid, 4-borono-, 1-[11-[(1-oxo-2-propenyl)oxy]undecyl] ester, polymer with N-butyl-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 698360-06-4

CMF C21 H31 B O6



CM 2

CRN 2565-18-6

CMF C7 H13 N O



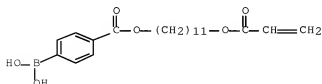
RN 698360-92-8 ZCAPLUS

CN 2-Propenoic acid, polymer with 11-[(1-oxo-2-propenyl)oxy]undecyl 4-boronobenzoate (9CI) (CA INDEX NAME)

CM 1

CRN 698360-06-4

CMF C21 H31 B O6

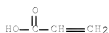


10/596571

CM 2

CRN 79-10-7

CMF C3 H4 O2



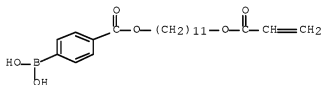
RN 698360-95-1 ZCAPLUS

CN Benzoic acid, 4-borono-, 1-[11-[(1-oxo-2-propenyl)oxy]undecyl] ester, polymer with 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid monosodium salt (9CI) (CA INDEX NAME)

CM 1

CRN 698360-06-4

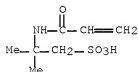
CMF C21 H31 B O6



CM 2

CRN 5165-97-9

CMF C7 H13 N O4 S . Na



● Na

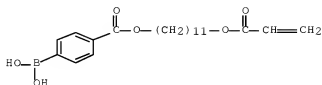
RN 698360-98-4 ZCAPLUS

CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride, polymer with 11-[(1-oxo-2-propenyl)oxy]undecyl 4-boronobenzoate and 2-propenamide (9CI) (CA INDEX NAME)

CM 1

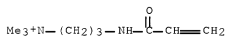
10/596571

CRN 698360-06-4
CMF C21 H31 B O6



CM 2

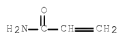
CRN 45021-77-0
CMF C9 H19 N2 O . Cl



● Cl⁻

CM 3

CRN 79-06-1
CMF C3 H5 N O

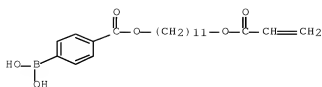


RN 698361-01-2 ZCAPLUS
CN Benzoic acid, 4-borono-, 1-[11-[(1-oxo-2-propenyl)oxy]undecyl] ester, polymer with 1-ethenyl-2-pyrrolidinone (9CI) (CA INDEX NAME)

CM 1

CRN 698360-06-4
CMF C21 H31 B O6

10/596571



CM 2

CRN 88-12-0

CMF C6 H9 N O



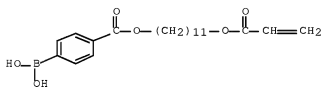
RN 698361-03-4 ZCAPLUS

CN 1-Propanaminium, N,N-dimethyl-N-[3-[(2-methyl-1-oxo-2-propenyl)amino]propyl]-3-sulfo-, inner salt, polymer with 11-[(1-oxo-2-propenyl)oxy]undecyl 4-boronobenzoate (9CI) (CA INDEX NAME)

CM 1

CRN 698360-06-4

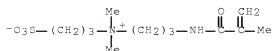
CMF C21 H31 B O6



CM 2

CRN 5205-95-8

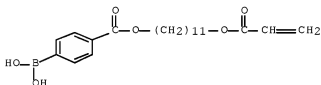
CMF C12 H24 N2 O4 S



RN 698361-05-6 ZCAPLUS
 CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride,
 polymer with 11-[(1-oxo-2-propenyl)oxy]undecyl 4-boronobenzoate (9CI) (CA
 INDEX NAME)

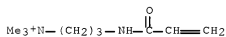
CM 1

CRN 698360-06-4
 CMF C21 H31 B O6



CM 2

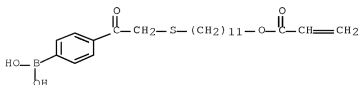
CRN 45021-77-0
 CMF C9 H19 N2 O . Cl



RN 698361-10-3 ZCAPLUS
 CN 1-Propanaminium, N,N,N-trimethyl-3-[(1-oxo-2-propenyl)amino]-, chloride,
 polymer with 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl 2-propenoate
 and 1-(1-oxo-2-propenyl)-2,5-pyrrolidinedione, graft (9CI) (CA INDEX
 NAME)

CM 1

CRN 698358-86-0
 CMF C22 H33 B O5 S

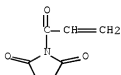


10/596571

CM 2

CRN 56905-55-6

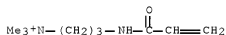
CMF C7 H7 N O3



CM 3

CRN 45021-77-0

CMF C9 H19 N2 O . Cl



● Cl⁻

RN 698382-85-3 ZCAPLUS

CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester, polymer with oxirane, methyl ether, graft (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1

CMF C H4 O



CM 2

CRN 698382-84-2

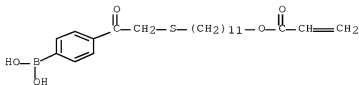
CMF (C22 H33 B O5 S . C2 H4 O)x

CCI PMS

CM 3

10/596571

CRN 698358-86-0
CMF C22 H33 B O5 S



CM 4

CRN 75-21-8
CMF C2 H4 O



IT 698358-73-5P 698358-86-0P 698359-11-4P
698359-23-8P 698359-33-0P 698359-82-9P
698359-88-5P 698360-02-0P 698360-06-4P
698360-09-7P

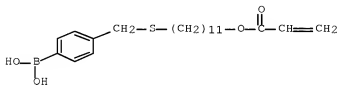
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(preparation and polymerization; polymeric boronic acid-pendant derivs. as lipase

inhibitors for treatment of obesity)

RN 698358-73-5 ZCAPLUS

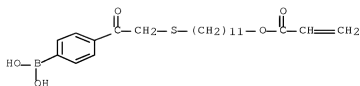
CN 2-Propenoic acid, 11-[(4-boronophenyl)methyl]thio]undecyl ester (9CI)
(CA INDEX NAME)



RN 698358-86-0 ZCAPLUS

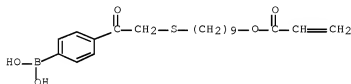
CN 2-Propenoic acid, 11-[[2-(4-boronophenyl)-2-oxoethyl]thio]undecyl ester (9CI) (CA INDEX NAME)

10/596571



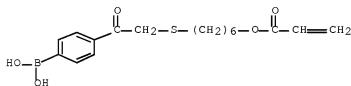
RN 698359-11-4 ZCAPLUS

CN 2-Propenoic acid, 9-[2-(4-boronophenyl)-2-oxoethyl]thiononyl ester (9CI)
(CA INDEX NAME)



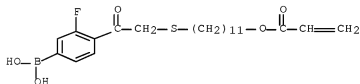
RN 698359-23-8 ZCAPLUS

CN 2-Propenoic acid, 6-[2-(4-boronophenyl)-2-oxoethyl]thiohexyl ester (9CI)
(CA INDEX NAME)



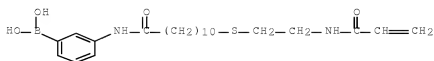
RN 698359-33-0 ZCAPLUS

CN 2-Propenoic acid, 11-[2-(4-borono-2-fluorophenyl)-2-oxoethyl]thioundecyl ester (9CI) (CA INDEX NAME)



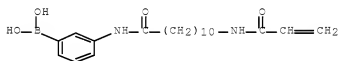
RN 698359-82-9 ZCAPLUS

CN Boronic acid, [3-[[1-oxo-11-[[2-[(1-oxo-2-propenyl)amino]ethyl]thio]undecyl]amino]phenyl]- (9CI) (CA INDEX NAME)



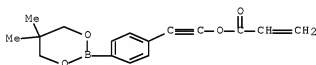
RN 698359-88-5 ZCAPLUS

CN Boronic acid, [3-[[[1-oxo-11-[(1-oxo-2-propenyl)amino]undecyl]amino]phenyl]- (9CI) (CA INDEX NAME)



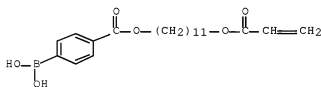
RN 698360-02-0 ZCAPLUS

CN 2-Propenoic acid, 2-[4-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)phenyl]ethynyl ester (CA INDEX NAME)



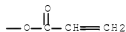
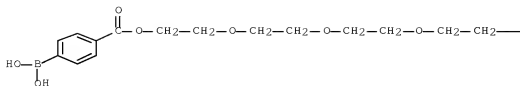
RN 698360-06-4 ZCAPLUS

CN Benzoic acid, 4-borono-, 1-[11-[(1-oxo-2-propenyl)oxy]undecyl] ester (9CI) (CA INDEX NAME)



RN 698360-09-7 ZCAPLUS

CN Benzoic acid, 4-borono-, 1-(13-oxo-3,6,9,12-tetraoxapentadec-14-en-1-yl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 23 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2004:308866 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 141:42740

TITLE: Glucose-responsive polymer gel bearing phenylborate derivative as a glucose-sensing moiety operating at the physiological pH

AUTHOR(S): Matsumoto, Akira; Yoshida, Ryo; Kataoka, Kazunori

CORPORATE SOURCE: Department of Materials Science and Engineering, Graduate School of Engineering, The University of Tokyo, Bunkyo, Tokyo, 113-8656, Japan

SOURCE: Biomacromolecules (2004), 5(3), 1038-1045

CODEN: BOMAF6; ISSN: 1525-7797

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The work attempts to prepare a totally synthetic, glucose-responsive polymer gel bearing a phenylborate derivative as a sensor moiety to glucose, for future use as a self-regulated insulin delivery system. The mol. strategies to enable the system to be operated under physiol. conditions (pH 7.4, 37 °C) were presented that involved the use of a novel phenylborate derivative {4-(1,6-dioxo-2,5-diaza-7-oxamyl) phenylboronic acid: DDOPBA} possessing an appreciably low pKa (.apprx.7.8), the adoption of poly(N-isopropylmethacrylamide) (PNIPMAAm) for the main chain, which itself undergoes a sharp thermo-induced phase transition at its LCST around 40 °C, as well as the introduction of a carboxyl group of methacrylic acid as the third comonomer. Glucose-responsive behaviors of the obtained gels were evaluated based on the changes in the equilibrium swelling degree determined in the presence and the absence of glucose, for various pH and temperature conditions. As a consequence of the combined mol. effects, a sufficient sensitivity of the system was accomplished at physiol. pH and in the temperature range close to the physiol. condition such as 30 °C. Furthermore, the glucose-induced continuous volume changes of the gels were demonstrated under those conditions, which occurred in a remarkably concentration-dependent manner. In these expts., the critical glucose concns. to induce the gels' responses in the range of normoglycemic sugar level were observed. These observations may provide us with an excellent prospect for the use of the gel

10/596571

as a self-regulated, insulin-delivery system discretely switching the release at the normoglycemia.

IT 250592-06-4P 611239-49-7P 701922-47-6P
701922-49-8P 701922-51-2P

RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(glucose-responsive polymer gel bearing phenylborate derivative as a glucose-sensing moiety operating at the physiolo. pH)

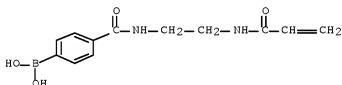
RN 250592-06-4 ZCAPLUS

CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4



CM 2

CRN 2210-25-5

CMF C6 H11 N O



RN 611239-49-7 ZCAPLUS

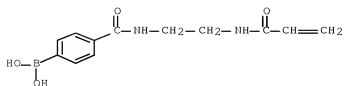
CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with 2-methyl-N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4

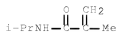
10/596571



CM 2

CRN 13749-61-6

CMF C7 H13 N O



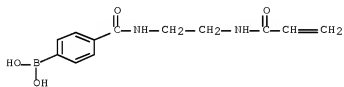
RN 701922-47-6 ZCAPLUS

CN Boronic acid, B-[4-[[[2-[(1-oxo-2-propen-1-yl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N,N'-methylenebis[2-propenamide] and N-(1-methylethyl)-2-propenamide (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4



CM 2

CRN 2210-25-5

CMF C6 H11 N O

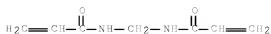


10/596571

CM 3

CRN 110-26-9

CMF C7 H10 N2 O2



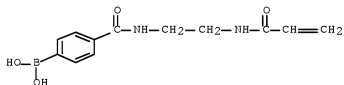
RN 701922-49-8 ZCAPLUS

CN Boronic acid, B-[4-[[[2-[(1-oxo-2-propen-1-yl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N,N'-methylenebis[2-propenamide] and 2-methyl-N-(1-methylethyl)-2-propenamide (CA INDEX NAME)

CM 1

CRN 250592-05-3

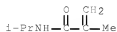
CMF C12 H15 B N2 O4



CM 2

CRN 13749-61-6

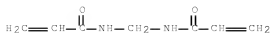
CMF C7 H13 N O



CM 3

CRN 110-26-9

CMF C7 H10 N2 O2



10/596571

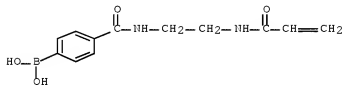
RN 701922-51-2 ZCAPLUS

CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N,N'-methylenebis[2-propenamide], 2-methyl-N-(1-methylethyl)-2-propenamide and 2-methyl-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4



CM 2

CRN 13749-61-6

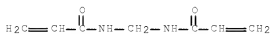
CMF C7 H13 N O



CM 3

CRN 110-26-9

CMF C7 H10 N2 O2



CM 4

CRN 79-39-0

CMF C4 H7 N O



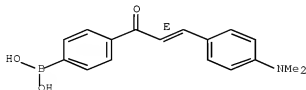
OS.CITING REF COUNT: 50 THERE ARE 50 CAPLUS RECORDS THAT CITE THIS RECORD (50 CITINGS)
 REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 24 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2003:1011575 ZCAPLUS Full-text
 DOCUMENT NUMBER: 140:195805
 TITLE: Noninvasive continuous monitoring of physiological glucose using a monosaccharide-sensing contact lens
 AUTHOR(S): Badugu, Ramachandram; Lakowicz, Joseph R.; Geddes, Chris D.
 CORPORATE SOURCE: Center for Fluorescence Spectroscopy, Department of Biochemistry and Molecular Biology, Medical Biotechnology Center, University of Maryland School of Medicine, Baltimore, MD, 21201, USA
 SOURCE: Analytical Chemistry (2004), 76(3), 610-618
 CODEN: ANCHAM; ISSN: 0003-2700
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB We have tested the feasibility of tear glucose sensing using a daily, disposable contact lens embedded with boronic acid-containing fluorophores as a potential alternative to current invasive glucose-monitoring techniques. Our findings show that our approach may, indeed, be suitable for the continuous monitoring of tear glucose levels in the range 50-500 μ M, which track blood glucose levels that are .apprx.5-10-fold higher. We compare the response of the boronic acid probes in the contact lens to solution-based measurements and can conclude that both the pH and polarity within the contact lens need to be considered with respect to choosing/designing and optimizing glucose-sensing probes for contact lenses.

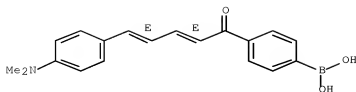
IT 661459-48-9 661459-49-0
 RL: ARU (Analytical role, unclassified); ANST (Analytical study) (noninvasive continuous monitoring of physiolo. glucose using monosaccharide-sensing contact lens)
 RN 661459-48-9 ZCAPLUS
 CN Boronic acid, [4-[(2E)-3-[4-(dimethylamino)phenyl]-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 661459-49-0 ZCAPLUS
 CN Boronic acid, [4-[(2E,4E)-5-[4-(dimethylamino)phenyl]-1-oxo-2,4-pentadienyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

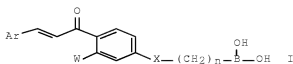


OS.CITING REF COUNT: 37 THERE ARE 37 CAPLUS RECORDS THAT CITE THIS
RECORD (37 CITINGS)
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 25 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:1006923 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:59511
TITLE: Preparation of boronic chalcone derivatives as
anticancer agents
INVENTOR(S): Khan, Saeed R.
PATENT ASSIGNEE(S): Johns Hopkins University, USA
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003106384	A2	20031224	WO 2003-US18962	20030612
WO 2003106384	A3	20040617		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003243594	A1	20031231	AU 2003-243594	20030612
US 20050176988	A1	20050811	US 2005-517781	20050420
US 7514579	B2	20090407		
US 20090227542	A1	20090910	US 2009-403288	20090312
PRIORITY APPLN. INFO.:			US 2002-388255P	P 20020613
			US 2003-444429P	P 20030203
			WO 2003-US18962	W 20030612
			US 2005-517781	A3 20050420

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 140:59511
GI



AB The present invention relates to novel boronic chalcone derivs. I (Ar = (un)substituted heteroaryl, etc.; W = H, etc.; X = Zn, etc.; n = 0 or any integer; Z = (un)substituted alkylene, etc.) which are useful as antitumor/anticancer agents. The activity of compds. of this invention against the growth of human breast cancer cell lines was demonstrated.

IT 562823-84-1P 562823-86-3P 562823-90-9P

562823-91-0P 562823-92-1P 562823-93-2P

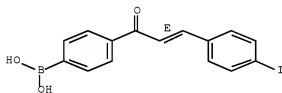
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of boronic chalcone derivs. as anticancer agents)

RN 562823-84-1 ZCAPLUS

CN Boronic acid, B-[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)

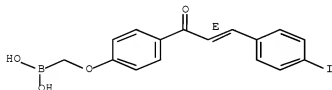
Double bond geometry as shown.



RN 562823-86-3 ZCAPLUS

CN Boronic acid, [[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propenyl]phenoxy]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

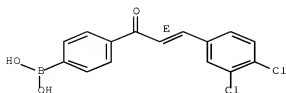


RN 562823-90-9 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

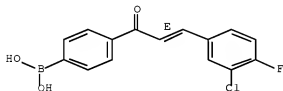
10/596571



RN 562823-91-0 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-chloro-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

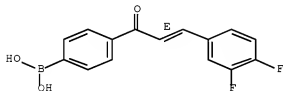
Double bond geometry as shown.



RN 562823-92-1 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-difluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

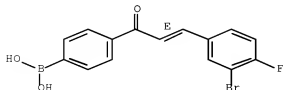
Double bond geometry as shown.



RN 562823-93-2 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-bromo-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



10/596571

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 26 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:852845 ZCAPLUS Full-text

DOCUMENT NUMBER: 139:330428

TITLE: Reactive mesogenic benzodithiophenes for liquid
crystal displaysINVENTOR(S): Farrand, Louise; Heeney, Martin; Tierny, Steven;
Giles, Mark; Thompson, Marcus; Shkunov, Maxim;
Sparrowe, David; McCulloch, Iain

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany

SOURCE: Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
EP 1357163	A1	20031029	EP 2003-6887	20030331
EP 1357163	B1	20060531		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AT 328050	T	20060615	AT 2003-6887	20030331
US 20030209692	A1	20031113	US 2003-421873	20030424
US 6913710	B2	20050705		
JP 2004002407	A	20040108	JP 2003-120754	20030424
PRIORITY APPLN. INFO.:			EP 2002-9083	A 20020424

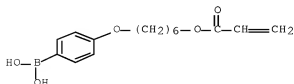
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB The invention relates to new reactive mesogenic benzodithiophene derivs.,
their use as semiconductors or charge transport materials, in optical,
electro-optical or electronic devices like for example liquid crystal
displays, optical films, organic field effect transistors (FET or OFET) for
thin film transistor liquid crystal displays and integrated circuit devices
such as RFID tags, electroluminescent devices in flat panel displays, and in
photovoltaic and sensor devices, and to a field effect transistor, light
emitting device or ID tag comprising the reactive mesogenic benzodithiophenes.

IT 615288-44-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of reactive mesogenic benzodithiophenes for liquid crystal
displays)

RN 615288-44-3 ZCAPLUS

CN 2-Propenoic acid, 6-(4-boronophenoxy)hexyl ester (9CI) (CA INDEX NAME)



10/596571

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(7 CITINGS)
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 27 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:643262 ZCAPLUS Full-text

DOCUMENT NUMBER: 139:312220

TITLE: Glucose-responsive polymer bearing a novel
phenylborate derivative as a glucose-sensing moiety
operating at physiological pH conditions

AUTHOR(S): Matsumoto, Akira; Ikeda, Syuhei; Harada, Atsushi;
Kataoka, Kazunori

CORPORATE SOURCE: Department of Materials Science and Engineering,
Graduate School of Engineering, The University of
Tokyo, Tokyo, 113-8656, Japan

SOURCE: Biomacromolecules (2003), 4(5), 1410-1416

CODEN: BOMAF6; ISSN: 1525-7797

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This study is devoted to the development of novel glucose-responsive polymers that operate under physiol. conditions (pH 7.4, 37 °C), aiming for future use in a self-regulated insulin delivery system to treat diabetes mellitus. The approach involves the use of a newly synthesized phenylborate derivative (4-(1,6-dioxo-2,5-diaza-7-oxamyl) phenylboronic acid, DDOPBA) possessing an appreciably low pKa (.apprx.7.8) as a glucose-sensing moiety, as well as the adoption of poly(N-isopropylmethacrylamide), PNIPMAAm, as the main chain that exhibits critical solution behavior in the range close to physiol. temperature. Glucose- and pH-dependent changes in the critical solution behavior of the resultant copolymers were investigated at varying temps., revealing definite glucose sensitivities near the physiol. conditions. Furthermore, DDOPBA moieties in the copolymers maintained constant apparent pKa values even when the temperature approaches the critical solution points of the main chain, indicating that spacing of the phenylborate moiety from the polymer backbone is a feasible way to minimize the microenvironment effect caused by a temperature-induced change in the hydration state of the polymer strands.

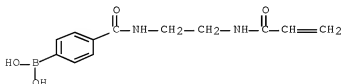
IT 250592-05-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(glucose-responsive polymer bearing a novel phenylborate derivative as a glucose-sensing moiety operating at physiol. pH)

RN 250592-05-3 ZCAPLUS

CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)



IT 250592-06-4P 611239-49-7P

RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use);

10/596571

BIOL (Biological study); PREP (Preparation); USES (Uses)
(glucose-responsive polymer bearing a novel phenylborate derivative as a
glucose-sensing moiety operating at physiol. pH)

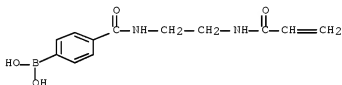
RN 250592-06-4 ZCAPLUS

CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with
N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4



CM 2

CRN 2210-25-5

CMF C6 H11 N O



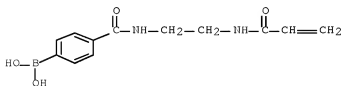
RN 611239-49-7 ZCAPLUS

CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with
2-methyl-N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4

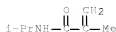


10/596571

CM 2

CRN 13749-61-6

CMF C7 H13 N O



OS.CITING REF COUNT: 52 THERE ARE 52 CAPLUS RECORDS THAT CITE THIS
RECORD (52 CITINGS)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 28 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:410905 ZCAPLUS Full-text

DOCUMENT NUMBER: 139:117464

TITLE: Design, Synthesis, and Evaluation of Novel
Boronic-Chalcone Derivatives as Antitumor Agents
AUTHOR(S): Kumar, Srinivas K.; Hager, Erin; Pettit, Catherine;
Gurulingappa, Hallur; Davidson, Nancy E.; Khan, Saeed
R.

CORPORATE SOURCE: Division of Experimental Therapeutics, Sidney Kimmel
Comprehensive Cancer Center at Johns Hopkins,
Baltimore, MD, 21231, USA

SOURCE: Journal of Medicinal Chemistry (2003), 46(14),
2813-2815

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:117464

AB A series of boronic-chalcone derivs., e.g. 4-IC6H4CH:CHCOC6H4B(OH)2-4, were
synthesized and tested for antitumor activity against human breast cancer cell
lines. The results show the boronic-chalcones are more toxic to breast cancer
cells compared to normal breast cells than other known chalcones.

IT 562823-84-1P 562823-86-3P 562823-90-9P
562823-91-0P 562823-92-1P 562823-93-2P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

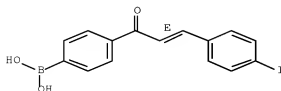
BIOL (Biological study); PREP (Preparation)

(design, synthesis, and evaluation of novel boronic-chalcone derivs. as
antitumor agents)

RN 562823-84-1 ZCAPLUS

CN Boronic acid, B-[4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propen-1-yl]phenyl]-
(CA INDEX NAME)

Double bond geometry as shown.

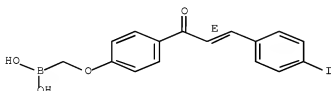


10/596571

RN 562823-86-3 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(4-iodophenyl)-1-oxo-2-propenyl]phenoxy)methyl]-
(9CI) (CA INDEX NAME)

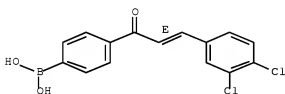
Double bond geometry as shown.



RN 562823-90-9 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

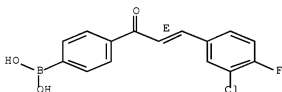
Double bond geometry as shown.



RN 562823-91-0 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-chloro-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

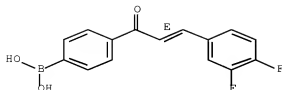
Double bond geometry as shown.



RN 562823-92-1 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3,4-difluorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

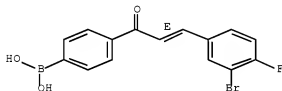
Double bond geometry as shown.



RN 562823-93-2 ZCAPLUS

CN Boronic acid, [4-[(2E)-3-(3-bromo-4-fluorophenyl)-1-oxo-2-propenyl]phenyl]-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 87 THERE ARE 87 CAPLUS RECORDS THAT CITE THIS RECORD (87 CITINGS)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 29 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2002:256773 ZCAPLUS Full-text

DOCUMENT NUMBER: 136:291357

TITLE: Detection of analytes in aqueous environments

INVENTOR(S): Colvin, Arthur E.

PATENT ASSIGNEE(S): Sensors for Medicine and Science, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 26 pp., Cont.-in-part of U. S. Ser. No. 632,624.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20020039793	A1	20020404	US 2001-920627	20010803
US 6794195	B2	20040921		
EP 1557422	A2	20050727	EP 2004-78499	20010803
EP 1557422	A3	20060705		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
US 20030003592	A1	20030102	US 2002-193246	20020712
US 20030008408	A1	20030109	US 2002-193244	20020712
US 20030013204	A1	20030116	US 2002-193245	20020712
US 20030013202	A1	20030116	US 2002-193249	20020712
IN 2003KN00229	A	20040918	IN 2003-KN229	20030224
US 20040229370	A1	20041118	US 2004-788264	20040301

10/596571

US 7060503	B2	20060613		
US 20060281185	A1	20061214	US 2006-448903	20060608
PRIORITY APPLN. INFO.:			US 2000-632624	A2 20000804
			EP 2001-956112	A3 20010803
			US 2001-920627	A1 20010803
			US 2004-788264	A1 20040301

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

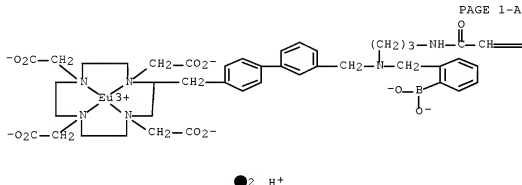
AB The invention concerns indicator mols. for detecting the presence or concentration of an analyte in a medium, such as a liquid, and to methods for achieving such detection. More particularly, the invention relates to copolymer macromols. containing relatively hydrophobic indicator component monomers, and hydrophilic monomers, such that the macromol. is capable of use in an aqueous environment.

IT 408306-50-3P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (detection of analytes in aqueous environments)

RN 408306-50-3 ZCAPLUS

CN Europate(3-), [2-[3'-[[[(2-boronophenyl)methyl][3-[(1-oxo-2-propenyl)amino]propyl]amino]methyl][1,1'-biphenyl]-4-yl]methyl]-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetato(6-)-κN1,κN4,κN7,κN10]-, dihydrogen, (SP-4-4)- (9CI) (CA INDEX NAME)



PAGE 1-B

==CH2

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 30 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2002:211081 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 137:134122

TITLE: Chalcone-analogue fluorescent probes for saccharides signaling using the boronic acid group

10/596571

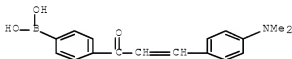
AUTHOR(S): DiCesare, Nicolas; Lakowicz, Joseph R.
CORPORATE SOURCE: Center for Fluorescence Spectroscopy, School of
Medicine, University of Maryland, Baltimore, MD,
21201, USA
SOURCE: Tetrahedron Letters (2002), 43(14), 2615-2618
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two new fluorescent probes based on 1,3-diphenylprop-2-en-1-one and on 1,5-diphenylpenta-2,4-dien-1-one structures are presented. Both probes possess one electron-donating dimethylamino group and one boronic acid group (electron-withdrawing group). The change between the neutral and the anionic form of the boronic acid group induced at high pH and/or in presence of sugar, induces optical changes for both probes. Spectroscopic data, pKa and dissociation consts. for different monosaccharides are presented and discussed in terms of sugar detection.

IT 406719-92-4 406719-94-6
RL: ARU (Analytical role, unclassified); DEV (Device component use); PRP (Properties); ANST (Analytical study); USES (Uses)
(chalcone-analog fluorescent probes for saccharides signaling using the boronic acid group)

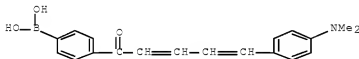
RN 406719-92-4 ZCAPLUS

CN Boronic acid, B-[4-[3-[4-(dimethylamino)phenyl]-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)



RN 406719-94-6 ZCAPLUS

CN Boronic acid, B-[4-[5-[4-(dimethylamino)phenyl]-1-oxo-2,4-pentadien-1-yl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 46 THERE ARE 46 CAPLUS RECORDS THAT CITE THIS RECORD (46 CITINGS)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 31 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2002:73583 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:275539

TITLE: New sensitive and selective fluorescent probes for fluoride using boronic acids

AUTHOR(S): DiCesare, Nicolas; Lakowicz, Joseph R.

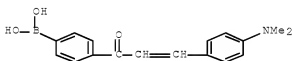
CORPORATE SOURCE: Center for Fluorescence Spectroscopy, University of Maryland, School of Medicine, Baltimore, MD, 21201, USA
 SOURCE: Analytical Biochemistry (2002), 301(1), 111-116
 CODEN: ANBCA2; ISSN: 0003-2697
 PUBLISHER: Academic Press
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB We report the spectroscopic characterization of six fluorescent probes for fluoride sensing and/or monitoring. All probes are based on the ability of the boronic acid group to interact with fluoride. The probes combine electron donor and withdrawing groups and involve the excited charge transfer mechanism. The change between the neutral form of the boronic acid group [R-B(OH)2], which is an electron withdrawing group, and the anionic trifluoro form [R-BF3-], which is an electron donating group, is at the origin of the different spectral changes observed for the investigated probes. Two probes are based on the stilbene structure where the boronic group in the 4 position is coupled with a cyano group, in one case, and the dimethylamino group in the other case, both at the 4' position. Another probe is based on the diphenyl-1,4-butadiene possessing the boronic acid group in the 4' position and a dimethylamino group in the 4' position. One probe is based on the diphenyloxazole structure having both the boronic acid and the dimethylamino groups in para positions. The two last probes reported are based on the benzalacetophenone (chalcone) structure, again coupling the boronic acid and dimethylamino groups. All probes show spectral shifts and/or intensity changes in the presence of fluoride resulting in most of the cases to a wavelength-ratiometric way for the detection and/or anal. of fluoride. Selectivity and stability consts. are also presented and discussed. (c) 2002 Academic Press.

IT 406719-92-4 406719-94-6
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (fluorescent probes for fluoride using boronic acids)

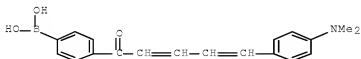
RN 406719-92-4 ZCAPLUS

CN Boronic acid, B-[4-[3-[4-(dimethylamino)phenyl]-1-oxo-2-propen-1-yl]phenyl]- (CA INDEX NAME)



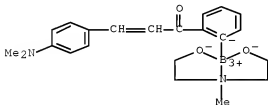
RN 406719-94-6 ZCAPLUS

CN Boronic acid, B-[4-[5-[4-(dimethylamino)phenyl]-1-oxo-2,4-pentadien-1-yl]phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 28 RECORD (51 CITINGS)
THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 32 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2001:186546 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 134:366929
TITLE: Synthesis, structure and spectroscopic characteristics
of 2'-boryl-4"-dimethylaminochalcones. Effect of an
intramolecular boron-oxygen coordinate bond to the
conjugated system
AUTHOR(S): Murafuji, Toshihiro; Sugimoto, Kenji; Yanagimoto,
Sachiko; Moriya, Tomokazu; Sugihara, Yoshikazu;
CORPORATE SOURCE: Mikata, Yuji; Kato, Masako; Yano, Shigenobu
Department of Chemistry, Faculty of Science, Yamaguchi
University, Yamaguchi, 753-8512, Japan
SOURCE: Heterocycles (2001), 54(2), 929-942
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:366929
AB 2'-Diethylboryl-4"-dimethylaminochalcone (1) and the related compds. (4)-(7)
bearing a dioxyboryl group in the 2'-position were synthesized, and the effect
of the intramol. B-O coordinate bond on the spectroscopic characteristics of
4"-dimethylaminochalcone chromophore was examined by comparison with 4"-
dimethylaminochalcone (2) using UV/visible and fluorescence spectra.
IT 340131-43-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 340131-43-3 ZCAPLUS
CN Boron, [2-[(2E)-3-[4-(dimethylamino)phenyl]-1-oxo-2-propenyl]phenyl][[2,2'-(
methylimino-κN)bis[ethanolato-κO]](2-)]-, (T-4)- (9CI) (CA
INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 33 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1999:747442 ZCAPLUS [Full-text](#)
DOCUMENT NUMBER: 131:352092
TITLE: Boronic acid group-containing monomers and
sugar-responsive polymers therefrom
INVENTOR(S): Kataoka, Kazunori; Harada, Atsushi; Ikeda, Shuichi;
Sakurai, Yasuhisa; Okano, Mitsuo; Aoyagi, Takao

10/596571

PATENT ASSIGNEE(S): Nippon Oil and Fats Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11322761	A	19991124	JP 1998-126082	19980508
JP 3867400	B2	20070110		

PRIORITY APPLN. INFO.: JP 1998-126082 19980508

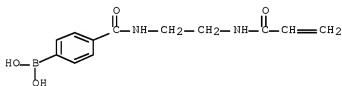
OTHER SOURCE(S): MARPAT 131:352092

AB The polymers, useful as artificial organs, chromatog. carriers, sugar-responsive gels, etc., contain units from H₂C:CR₁CONHR₂NHCOC₆H₄B(OH)₂ [I; R₁ = H, Me; R₂ = R₄O(R₃O)_nR₅, C₂-8 hydrocarbylene; R₃ = C₂-4 alkylene; R₄ = CH₂CH₂, COCH₂; R₅ = CH₂CH₂, CH₂CO; n = 1-200]. Thus, 4-HO₂CC₆H₄B(OH)₂ was chlorinated by SOCl₂, amidated by ethylenediamine, and condensed with acryloyl chloride to give 4-I (R₁ = R₂ = H), which was polymerized with N-isopropylacrylamide to give polymer. The polymer was soluble in phosphate buffer physiol. saline in the presence of ≤3 g/L glucose, while precipitated in the presence of ≥5 g/L glucose.

IT 250592-05-3P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of boronic acid group-containing monomers and their polymers responsive to sugars)

RN 250592-05-3 ZCAPLUS

CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)



IT 250592-06-4P
 RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of boronic acid group-containing monomers and their polymers responsive to sugars)

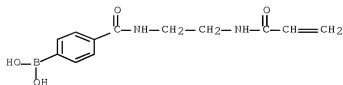
RN 250592-06-4 ZCAPLUS

CN Boronic acid, [4-[[[2-[(1-oxo-2-propenyl)amino]ethyl]amino]carbonyl]phenyl]-, polymer with N-(1-methylethyl)-2-propenamide (9CI) (CA INDEX NAME)

CM 1

CRN 250592-05-3

CMF C12 H15 B N2 O4



CM 2

CRN 2210-25-5
CMF C6 H11 N O



L41 ANSWER 34 OF 34 ZCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1999:422273 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 131:214326

TITLE: Structure and spectroscopic characteristics of
2'-diethylboryl-4''-dimethylaminochalcone bearing an
intramolecular boron-oxygen coordinate bond

AUTHOR(S): Murafuji, Toshihiro; Sugihara, Yoshikazu; Moriya,
Tomokazu; Mikata, Yuji; Yano, Shigenobu

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Yamaguchi
University, Yamaguchi City, 753-8512, Japan

SOURCE: New Journal of Chemistry (1999), 23(7), 683-685
CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB How formation of an intramol. coordinate bond affects mol. structure was
examined in the structural comparison of (E)-2'-diethylboryl-4''-
dimethylaminochalcone (1) and 2'-ethylenedioxyboryl-4''-dimethylaminochalcone
(2) with chloro{2-[(4-dimethylaminostyryl)carbonyl]phenyl}(4-
methylphenyl)bismuthane (3) and (E)-4''-dimethylaminochalcone (4). 1-4 Were
prepared and characterized spectroscopically and X-ray crystallog. structures
were determined for 1 and 4.

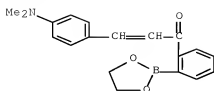
IT 243140-10-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 243140-10-5 ZCAPLUS

CN 2-Propen-1-one, 3-[4-(dimethylamino)phenyl]-1-[2-(1,3,2-dioxaborolan-2-
yl)phenyl]- (CA INDEX NAME)

10/596571



OS.CITING REF COUNT:	12	THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)
REFERENCE COUNT:	12	THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his full

(FILE 'HOME' ENTERED AT 10:56:09 ON 04 JAN 2010)

FILE 'REGISTRY' ENTERED AT 10:56:19 ON 04 JAN 2010

L1 STRUCTURE UPLOADED
 L2 50 SEA SSS SAM L1
 L3 STRUCTURE UPLOADED
 L4 46 SEA SSS SAM L3
 D SCA

FILE 'ZCAPLUS' ENTERED AT 11:10:35 ON 04 JAN 2010

E US2007-596751 /APPS
 L5 1 SEA SPE=ON ABB=ON PLU=ON US2007-596751 /AP
 D SCA
 SEL RN

FILE 'REGISTRY' ENTERED AT 12:10:52 ON 04 JAN 2010

L6 2 SEA SPE=ON ABB=ON PLU=ON (856849-32-6/BI OR 856849-35-9/BI)
 D SCA
 D STAT QUE L4
 L7 995 SEA SSS FUL L3
 SAVE TEMP L7 CHA751STR3L/A

FILE 'ZCAPLUS' ENTERED AT 12:14:15 ON 04 JAN 2010

L8 474 SEA SPE=ON ABB=ON PLU=ON L7
 L9 ANALYZE PLU=ON L8 1- RN HIT : 870 TERMS
 D
 SEL 1-10

FILE 'REGISTRY' ENTERED AT 12:15:16 ON 04 JAN 2010

L10 10 SEA SPE=ON ABB=ON PLU=ON (99349-68-5/RN OR 48150-45-4/RN OR
 152635-75-1/RN OR 172994-70-6/RN OR 136043-34-0/RN OR 99349-69-
 6/RN OR 159896-15-8/RN OR 136043-29-3/RN OR 219318-45-3/RN OR
 151169-68-5/RN)
 D SCA
 L11 STRUCTURE UPLOADED
 L12 1 SEA SUB=L7 SSS SAM L11
 D SCA
 L13 4 SEA SUB=L7 SSS FUL L11
 D SCA

FILE 'ZCAPLUS' ENTERED AT 12:23:31 ON 04 JAN 2010

L14 4 SEA SPE=ON ABB=ON PLU=ON L13

FILE 'REGISTRY' ENTERED AT 12:42:40 ON 04 JAN 2010

L15 STRUCTURE UPLOADED
 L16 4 SEA SUB=L7 SSS SAM L15
 D SCA
 L17 58 SEA SUB=L7 SSS FUL L15
 D SCA
 L18 STRUCTURE UPLOADED
 L19 2 SEA SUB=L17 SSS SAM L18
 L20 20 SEA SUB=L17 SSS FUL L18
 D SCA

FILE 'ZCAPLUS' ENTERED AT 12:53:51 ON 04 JAN 2010

10/596571

```

L21      20 SEA SPE=ON  ABB=ON  PLU=ON  L20
          D SCA

FILE 'REGISTRY' ENTERED AT 13:04:18 ON 04 JAN 2010
L22      STRUCTURE UPLOADED
L23      3 SEA SUB=L7 SSS SAM L22
          D SCA
L24      75 SEA SUB=L7 SSS FUL L22
          D SCA
L25      9 SEA SPE=ON  ABB=ON  PLU=ON  L24 AND B>1
          D SCA

FILE 'ZCAPLUS' ENTERED AT 13:09:11 ON 04 JAN 2010
L26      15 SEA SPE=ON  ABB=ON  PLU=ON  L24

FILE 'REGISTRY' ENTERED AT 13:09:44 ON 04 JAN 2010
          D SCA L20
L27      95 SEA SPE=ON  ABB=ON  PLU=ON  L20 OR L24

FILE 'ZCAPLUS' ENTERED AT 13:10:35 ON 04 JAN 2010
L28      34 SEA SPE=ON  ABB=ON  PLU=ON  L27

FILE 'REGISTRY' ENTERED AT 13:12:03 ON 04 JAN 2010
L29      STRUCTURE UPLOADED
L30      1 SEA SUB=L7 SSS SAM L29
L31      2 SEA SUB=L7 SSS FUL L29
          D SCA
L32      2 SEA SPE=ON  ABB=ON  PLU=ON  L31 AND L20

FILE 'ZCAPLUS' ENTERED AT 13:17:10 ON 04 JAN 2010
L33      5 SEA SPE=ON  ABB=ON  PLU=ON  L31
L34      4245 SEA SPE=ON  ABB=ON  PLU=ON  KHAN S7/AU, AUTH
L35      5 SEA SPE=ON  ABB=ON  PLU=ON  L7 AND L34
          D SCA
L36      10335 SEA SPE=ON  ABB=ON  PLU=ON  BORONIC ACID?/BI
L37      4 SEA SPE=ON  ABB=ON  PLU=ON  L34 AND L36

FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 13:19:34 ON 04 JAN 2010
L38      10 SEA SPE=ON  ABB=ON  PLU=ON  L34 AND BORONIC ACID?

FILE 'REGISTRY' ENTERED AT 13:20:06 ON 04 JAN 2010

FILE 'ZCAPLUS' ENTERED AT 13:20:08 ON 04 JAN 2010
          D STAT QUE L35
          D STAT QUE L37
L39      6 SEA SPE=ON  ABB=ON  PLU=ON  L35 OR L37

FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 13:20:25 ON 04 JAN 2010
          D STAT QUE L38

FILE 'ZCAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 13:20:37 ON 04
JAN 2010
L40      8 DUP REM L39 L38 (8 DUPLICATES REMOVED)
          ANSWERS '1-6' FROM FILE ZCAPLUS
          ANSWERS '7-8' FROM FILE MEDLINE
          D IBIB ABS HITIND HITSTR L40 1-6
          D IALL L40 7-8

FILE 'REGISTRY' ENTERED AT 13:21:57 ON 04 JAN 2010

```

FILE 'ZCAPLUS' ENTERED AT 13:22:00 ON 04 JAN 2010
D STAT QUE L14
D IBIB ABS HITSTR L14 1-4

FILE 'REGISTRY' ENTERED AT 13:22:35 ON 04 JAN 2010

FILE 'ZCAPLUS' ENTERED AT 13:22:37 ON 04 JAN 2010
D STAT QUE L21
D STAT QUE L26
D STAT QUE L33

L41 34 SEA SPE=ON ABB=ON PLU=ON L21 OR L26 OR L33
D IBIB ABS HITSTR L41 1-34

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0
DICTIONARY FILE UPDATES: 3 JAN 2010 HIGHEST RN 1200115-43-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

FILE ZCAPLUS

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN. Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS is
strictly prohibited.

FILE COVERS 1907 - 4 Jan 2010 VOL 152 ISS 2
FILE LAST UPDATED: 3 Jan 2010 (20100103/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE MEDLINE

FILE LAST UPDATED: 2 Jan 2010 (20100102/UP). FILE COVERS 1949 TO DATE.

MEDLINE and LMEDLINE have been updated with the 2010 Medical Subject Headings (MeSH) vocabulary and tree numbers from the U.S. National Library of Medicine (NLM). Additional information is available at

http://www.nlm.nih.gov/pubs/techbull/nd09/nd09_medline_data_changes_2010.

See HELP RLOAD for details.

MEDLINE was last reloaded on February 21, 2009.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

FILE EMBASE

FILE COVERS 1974 TO 4 Jan 2010 (20100104/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE BIOSIS

FILE COVERS 1926 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 30 December 2009 (20091230/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX

FILE LAST UPDATED: 22 DEC 2009 <20091222/UP>

MOST RECENT UPDATE: 200982 <200982/DW>

DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> Now containing more than 1.5 million chemical structures in DCR <<<

>>> IPC, ECLA, US National Classifications and Japanese F-Terms and FI-Terms have been updated with reclassifications to end of September 2009.

No update date (UP) has been created for the reclassified documents, but they can be identified by specific update codes (see HELP CLA for details) <<<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:

http://www.stn-international.com/stn_guide.html

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE

<http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate>

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:

http://www.stn-international.com/DWPIAnaVist2_0608.html

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> Japanese FI-TERM thesaurus in field /FCL added --> see NEWS <<<

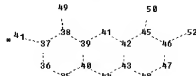
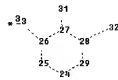
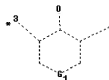
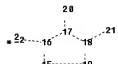
Uploading L3.str



6_2



56



chain nodes :

11 12 13 14 20 21 22 23 31 32 49 50 51 52 56

ring nodes :

1 2 3 4 5 6 15 16 17 18 19 24 25 26 27 28 29 35 36 37 38 39
40 41 42 43 44 45 46 47 48

ring/chain nodes :

7 8 9

chain bonds :

11-12 11-13 13-14 16-22 17-20 18-21 23-26 27-31 28-32 37-51 38-49 45-50
46-52

10/596571

ring/chain bonds :

7-8 7-9

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-19 16-17 17-18 18-19 24-25 24-29 25-26

26-27 27-28 28-29 35-36 35-40 36-37 37-38 38-39 39-40 39-41 40-44 41-42
42-43 42-45

43-44 43-48 45-46 46-47 47-48

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 11-12 11-13 13-14 15-16 15-19 16-17
16-22 17-18 17-20 18-19 18-21 23-26 24-25 24-29 25-26 26-27 27-28 27-31

28-29 28-32

35-36 35-40 36-37 37-38 37-51 38-39 38-49 39-40 39-41 40-44 41-42 42-43

42-45 43-44 43-48

45-46 45-50 46-47 46-52 47-48

G1:C,N

G2:[*1],[*2],[*3],[*4]

Connectivity :

15:2 E exact RC ring/chain 16:3 E exact RC ring/chain 17:3 E exact RC ring/chain

18:3 E exact RC ring/chain 19:2 E exact RC ring/chain 20:1 E exact RC ring/chain

21:2 X maximum

RC ring/chain 22:2 E exact RC ring/chain 23:2 E exact RC ring/chain 25:2 E exact
RC ring/chain

26:3 E exact RC ring/chain 27:3 E exact RC ring/chain 28:3 E exact RC ring/chain

29:2 E exact

RC ring/chain 31:1 E exact RC ring/chain 32:2 X maximum RC ring/chain 38:3 E

exact RC ring/chain

45:3 E exact RC ring/chain 46:3 E exact RC ring/chain 49:1 E exact RC ring/chain

50:1 E exact

RC ring/chain 51:2 E exact RC ring/chain 52:2 X maximum RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS

12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS

21:CLASS

22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:CLASS

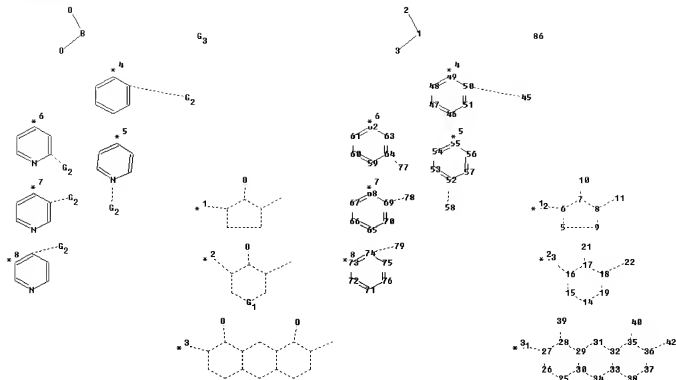
32:CLASS 35:Atom

36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom

45:Atom 46:Atom

47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:CLASS 56:CLASS

Uploading L11.str



chain nodes :

10 11 12 13 21 22 39 40 41 42 45 58 77 78 79 86

ring nodes :

5 6 7 8 9 14 15 16 17 18 19 25 26 27 28 29 30 31 32 33 34 35
 36 37 38 46 47 48 49 50 51 52 53 54 55 56 57 59 60 61 62 63 64
 65 66 67 68
 69 70 71 72 73 74 75 76

ring/chain nodes :

1 2 3

chain bonds :

6-12 7-10 8-11 13-16 17-21 18-22 27-41 28-39 35-40 36-42 45-50 52-58
 64-77 69-78 74-79

ring/chain bonds :

1-2 1-3

ring bonds :

5-6 5-9 6-7 7-8 8-9 14-15 14-19 15-16 16-17 17-18 18-19 25-26 25-30
 26-27 27-28 28-29 29-30 29-31 30-34 31-32 32-33 32-35 33-34 33-38 35-36
 36-37 37-38 46-47
 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 56-57 59-60
 59-64 60-61
 61-62 62-63 63-64 65-66 65-70 66-67 67-68 68-69 69-70 71-72 71-76 72-73
 73-74 74-75
 75-76

exact/norm bonds :

1-2 1-3 5-6 5-9 6-7 6-12 7-8 7-10 8-9 8-11 13-16 14-15 14-19 15-16
 16-17 17-18 17-21 18-19 18-22 25-26 25-30 26-27 27-28 27-41 28-29 28-39
 29-30 29-31 30-34
 31-32 32-33 32-35 33-34 33-38 35-36 35-40 36-37 36-42 37-38 45-50 52-58
 64-77 69-78
 74-79

normalized bonds :

46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 56-57
 59-60 59-64 60-61 61-62 62-63 63-64 65-66 65-70 66-67 67-68 68-69 69-70

10/596571

71-72 71-76
72-73 73-74 74-75 75-76

G1:C,N

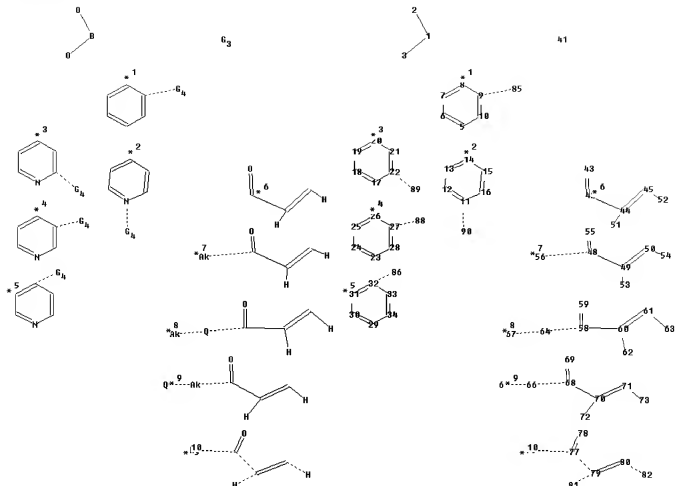
G2:[*1],[*2],[*3]

G3:[*4],[*5],[*6],[*7],[*8]

Match level :

1:CLASS 2:CLASS 3:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS
12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS
22:CLASS
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom
34:Atom 35:Atom
36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:CLASS
46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom
58:CLASS 59:CLASS
60:CLASS 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom
69:Atom
70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:CLASS 78:CLASS
79:CLASS 86:CLASS

Uploading L15.str



chain nodes :

41 42 43 44 45 48 49 50 51 52 53 54 55 56 58 59 60 61 62 63 64
65 66 67 68 69 70 71 72 73 76 77 78 79 80 81 82 85 86 88 89 90

ring nodes :

5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
27 28 29 30 31 32 33 34

ring/chain nodes :

1 2 3

chain bonds :

9-85 11-90 22-89 27-88 32-86 42-43 42-44 44-45 44-51 45-52 48-49 48-55
48-56 49-50 49-53 50-54 58-59 58-60 58-64 60-61 60-62 61-63 64-67 65-66
66-68 68-69
68-70 70-71 70-72 71-73 76-77 77-78 77-79 79-80 79-81 80-82

ring/chain bonds :

1-2 1-3

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-18
17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 29-30
29-34 30-31 31-32
32-33 33-34

exact/norm bonds :

1-2 1-3 9-85 11-90 22-89 27-88 32-86 42-43 48-55 48-56 58-59 58-64 64-67

65-66 66-68 68-69 76-77 77-78 77-79 79-81 80-82

exact bonds :

42-44 44-45 44-51 45-52 48-49 49-50 49-53 50-54 58-60 60-61 60-62 61-63

10/596571

68-70 70-71 70-72 71-73 79-80

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-18
17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28 29-30
29-34 30-31 31-32
32-33 33-34

G1:C,N

G3:[*1],[*2],[*3],[*4],[*5]

G4:[*6],[*7],[*8],[*9],[*10]

Connectivity :

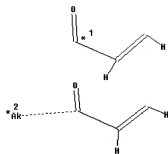
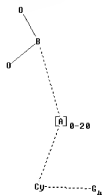
45:2 X maximum RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom 20:Atom
21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom
34:Atom 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 48:CLASS 49:CLASS
50:CLASS 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 58:CLASS 59:CLASS 60:CLASS
61:CLASS 62:CLASS
63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS
71:CLASS 72:CLASS
73:CLASS 76:Atom 77:CLASS 78:CLASS 79:CLASS 80:CLASS 81:CLASS 82:CLASS
85:CLASS 86:CLASS
88:CLASS 89:CLASS 90:CLASS

Uploading L18.str

10/596571



10/596571

G1:C,N

G4:[*1],[*2],[*3],[*4],[*5]

Connectivity :

8:2 X maximum RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 11:CLASS 12:CLASS

13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS

22:CLASS 23:CLASS

24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

32:CLASS 33:CLASS

34:CLASS 35:CLASS 36:CLASS 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS

44:CLASS 45:CLASS

48:Atom 49:CLASS 51:CLASS

Generic attributes :

48:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 48: Limited

C,C6

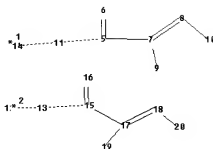
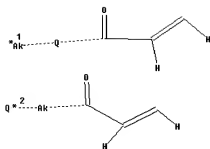
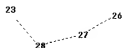
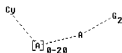
N,N0-1

O,O0

S,S0

Uploading L22.str

10/596571



```

chain nodes :
5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 23 26 27 28
ring/chain nodes :
1 2 3
chain bonds :
5-6 5-7 5-11 7-8 7-9 8-10 11-14 12-13 13-15 15-16 15-17 17-18 17-19
18-20 23-28 26-27 27-28
ring/chain bonds :
1-2 1-3
exact/norm bonds :
1-2 1-3 5-6 5-11 11-14 12-13 13-15 15-16 23-28 26-27 27-28
exact bonds :
5-7 7-8 7-9 8-10 15-17 17-18 17-19 18-20

```

G1:C,N

G2:[*1],[*2]

```

Match level :
1:CLASS 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS
23:Atom 26:CLASS 27:CLASS 28:CLASS

```

10/596571

Generic attributes :

23:

Saturation : Unsaturated

Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 23: Limited

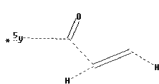
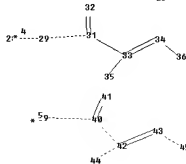
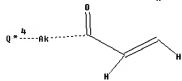
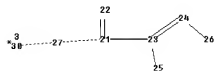
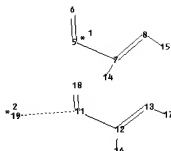
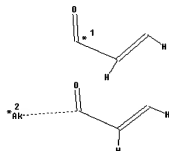
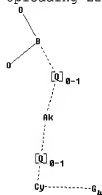
C,C6

N,N0-1

O,O0

S,S0

Uploading L29.str



chain nodes :

10/596571

```
5  6  7  8  11 12 13 14 15 16 17 18 19 21 22 23 24 25 26 27 28 29
30 31 32 33 34 35 36 39 40 41 42 43 44 45 48 49 51 52 55
ring/chain nodes :
1  2  3
chain bonds :
1-52  5-6  5-7  7-8  7-14  8-15  11-12  11-18  11-19  12-13  12-16  13-17  21-22
21-23  21-27  23-24  23-25  24-26  27-30  28-29  29-31  31-32  31-33  33-34  33-35
34-36  39-40
40-41  40-42  42-43  42-44  43-45  48-49  48-55  51-52  51-55
ring/chain bonds :
1-2  1-3
exact/norm bonds :
1-2  1-3  1-52  5-6  11-18  11-19  21-22  21-27  27-30  28-29  29-31  31-32  39-40
40-41  40-42  42-44  43-45  48-49  48-55  51-52  51-55
exact bonds :
5-7  7-8  7-14  8-15  11-12  12-13  12-16  13-17  21-23  23-24  23-25  24-26  31-33
33-34  33-35  34-36  42-43
```

G1:C,N

G4:[*1],[*2],[*3],[*4],[*5]

```
Connectivity :
8:2 X maximum RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS
22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS
34:CLASS 35:CLASS 36:CLASS 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS
44:CLASS 45:CLASS
48:Atom 49:CLASS 51:CLASS 52:CLASS 55:CLASS
Generic attributes :
48:
Saturation      : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
```

```
Element Count :
Node 48: Limited
C,C6
N,N0-1
O,O0
S,S0
```

=>